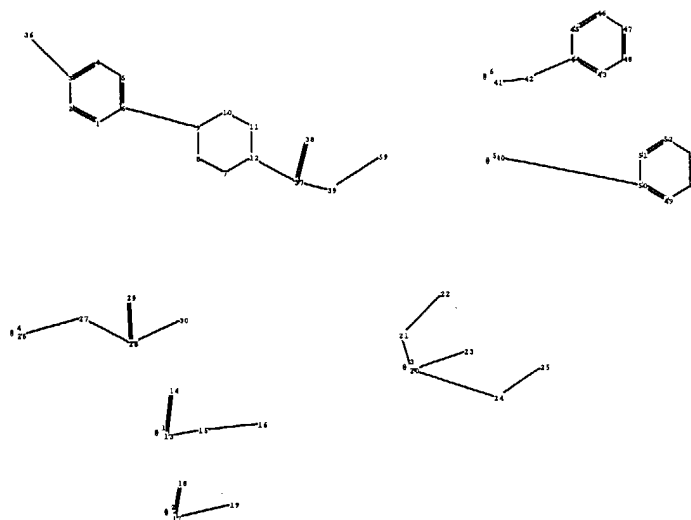
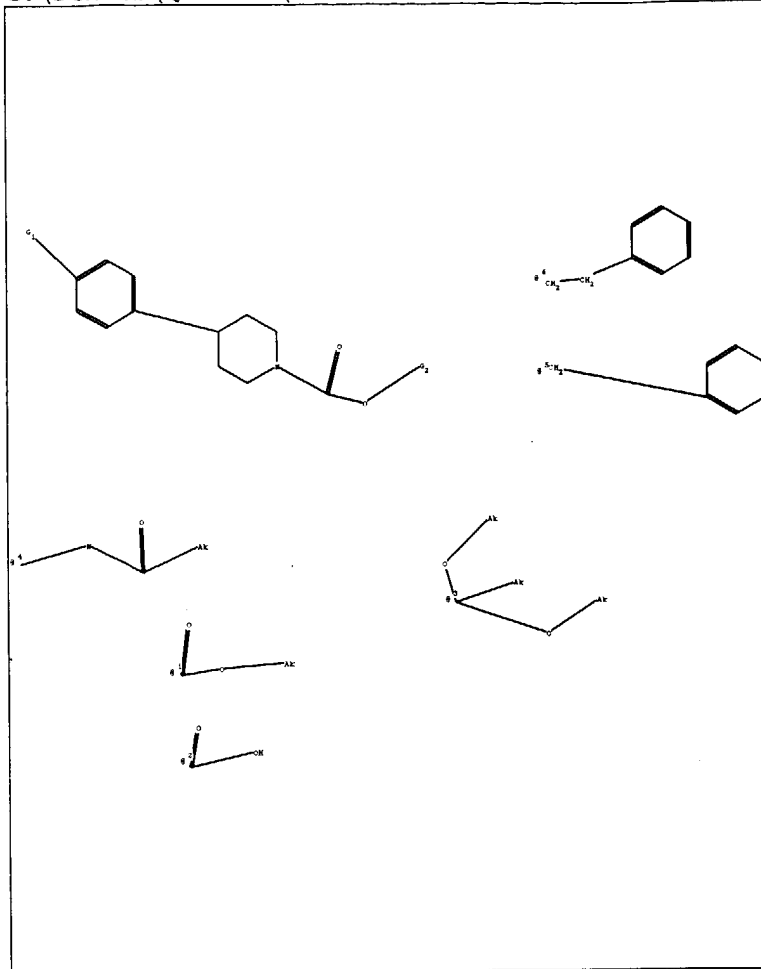


c:\stnweb\Queries\4.str



```

chain nodes :
13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 36 37 38 39
40 41 42 59
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 43 44 45 46 47 48 49 50 51 52 53 54
chain bonds :
3-36 6-9 12-37 13-14 13-15 15-16 17-18 17-19 20-21 20-23 20-24 21-22 24-25
26-27 27-28 28-29 28-30 37-38 37-39 39-59 40-50 41-42 42-44
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 43-44 43-48 44-45
45-46 46-47 47-48 49-50 49-54 50-51 51-52 52-53 53-54
exact/norm bonds :
3-36 7-8 7-12 8-9 9-10 10-11 11-12 12-37 13-14 13-15 15-16 20-21 20-23 20-24
21-22 24-25 26-27 27-28 28-29 28-30 37-38 37-39 39-59
exact bonds :
6-9 40-50 41-42 42-44
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 17-18 17-19 43-44 43-48 44-45 45-46 46-47 47-48
49-50 49-54 50-51 51-52 52-53 53-54
isolated ring systems :
containing 1 : 7 : 43 : 49 :

```

G1:CN,[\*1],[\*2],[\*3],[\*4]

G2:Ph,Ak,[\*5],[\*6]

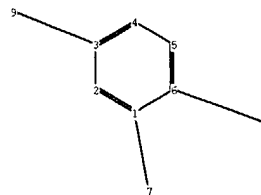
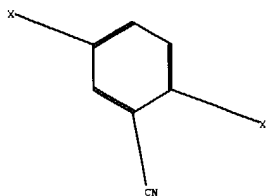
Match level :

```

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS 20:CLASS
21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS
30:CLASS 36:CLASS 37:CLASS 38:CLASS 39:CLASS 40:CLASS 41:CLASS 42:CLASS 43:Atom
44:Atom 45:Atom 46:Atom 47:Atom 48:Atom 49:Atom 50:Atom 51:Atom 52:Atom 53:Atom
54:Atom 59:CLASS

```

c:\stnweb\Queries\6.str



chain nodes :

7 8 9

ring nodes :

1 2 3 4 5 6

chain bonds :

1-7 3-9 6-8

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6

exact bonds :

1-7 3-9 6-8

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

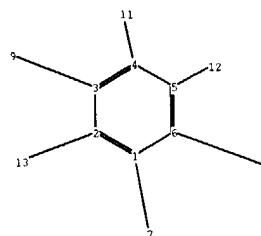
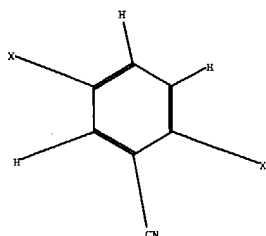
isolated ring systems :

containing 1 :

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS

C:\stnweb\Queries\1.str



chain nodes :

7 8 9 11 12 13

ring nodes :

1 2 3 4 5 6

chain bonds :

1-7 2-13 3-9 4-11 5-12 6-8

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6

exact bonds :

1-7 2-13 3-9 4-11 5-12 6-8

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

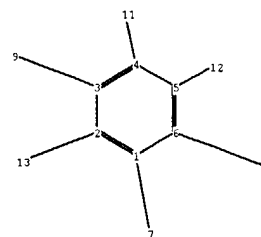
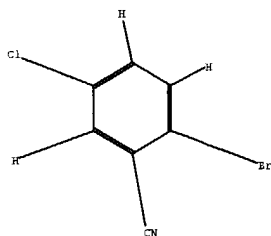
isolated ring systems :

containing 1 :

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 11:CLASS  
12:CLASS 13:CLASS

C:\stnweb\Queries\5a.str



chain nodes :

7 8 9 11 12 13

ring nodes :

1 2 3 4 5 6

chain bonds :

1-7 2-13 3-9 4-11 5-12 6-8

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6

exact bonds :

1-7 2-13 3-9 4-11 5-12 6-8

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

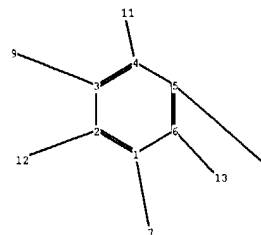
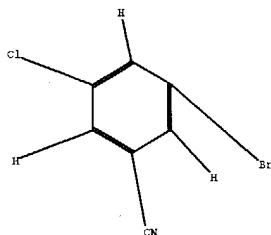
isolated ring systems :

containing 1 :

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 11:CLASS  
12:CLASS 13:CLASS

C:\stnweb\Queries\6.str



chain nodes :

7 8 9 11 12 13

ring nodes :

1 2 3 4 5 6

chain bonds :

1-7 2-12 3-9 4-11 5-8 6-13

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6

exact bonds :

1-7 2-12 3-9 4-11 5-8 6-13

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

isolated ring systems :

containing 1 :

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 11:CLASS  
12:CLASS 13:CLASS

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NEWS 1 Web Page URLs for STN Seminar Schedule - N. America  
NEWS 2 "Ask CAS" for self-help around the clock  
NEWS 3 Jul 12 BEILSTEIN enhanced with new display and select options,  
 resulting in a closer connection to BABS  
NEWS 4 AUG 02 IFIPAT/IFIUDB/IFICDB reloaded with new search and display  
 fields  
NEWS 5 AUG 02 CAlus and CA patent records enhanced with European and Japan  
 Patent Office Classifications  
NEWS 6 AUG 02 The Analysis Edition of STN Express with Discover!  
 (Version 7.01 for Windows) now available  
NEWS 7 AUG 27 BIOCOMMERCE: Changes and enhancements to content coverage  
NEWS 8 AUG 27 BIOTECHABS/BIOTECHDS: Two new display fields added for legal  
 status data from INPADOC  
NEWS 9 SEP 01 INPADOC: New family current-awareness alert (SDI) available  
NEWS 10 SEP 01 New pricing for the Save Answers for SciFinder Wizard within  
 STN Express with Discover!  
NEWS 11 SEP 01 New display format, HITSTR, available in WPIDS/WPINDEX/WPIX  
NEWS 12 SEP 14 STN Patent Forum to be held October 13, 2004, in Iselin, NJ  
NEWS 13 SEP 27 STANDARDS will no longer be available on STN  
NEWS 14 SEP 27 SWETSCAN will no longer be available on STN  
NEWS 15 SEP 30 STN downtime scheduled October 2-3, 2004

NEWS EXPRESS JULY 30 CURRENT WINDOWS VERSION IS V7.01, CURRENT  
 MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),  
 AND CURRENT DISCOVER FILE IS DATED 11 AUGUST 2004

NEWS HOURS STN Operating Hours Plus Help Desk Availability  
NEWS INTER General Internet Information  
NEWS LOGIN Welcome Banner and News Items  
NEWS PHONE Direct Dial and Telecommunication Network Access to STN  
NEWS WWW CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that  
 specific topic.

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\* \* \* \* \* STN Columbus \* \* \* \* \*

FILE 'HOME' ENTERED AT 14:06:26 ON 01 OCT 2004

=> file req

COST IN U.S. DOLLARS

SINCE FILE TOTAL  
 ENTRY SESSION

FULL ESTIMATED COST

0.21 0.21

FILE 'REGISTRY' ENTERED AT 14:06:32 ON 01 OCT 2004

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STRUCTURE FILE UPDATES: 29 SEP 2004 HIGHEST RN 754169-63-6

DICTIONARY FILE UPDATES: 29 SEP 2004 HIGHEST RN 754169-63-6

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:  
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=>

L1 STRUCTURE UPLOADED

=> s l1

SAMPLE SEARCH INITIATED 14:13:31 FILE 'REGISTRY'  
 SAMPLE SCREEN SEARCH COMPLETED - 37 TO ITERATE

100.0% PROCESSED 37 ITERATIONS 1 ANSWERS  
 SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
 BATCH \*\*COMPLETE\*\*  
 PROJECTED ITERATIONS: 376 TO 1104  
 PROJECTED ANSWERS: 1 TO 80

L2 1 SEA SSS SAM L1

=> s l1 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS  
 DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y  
 FULL SEARCH INITIATED 14:13:36 FILE 'REGISTRY'  
 FULL SCREEN SEARCH COMPLETED - 821 TO ITERATE

100.0% PROCESSED 821 ITERATIONS 19 ANSWERS  
 SEARCH TIME: 00.00.01

L3 19 SEA SSS FUL L1

=> file hcaplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	160.04	160.25

FILE 'HCAPLUS' ENTERED AT 14:13:42 ON 01 OCT 2004  
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FILE COVERS 1907 - 1 Oct 2004 VOL 141 ISS 15  
FILE LAST UPDATED: 30 Sep 2004 (20040930/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l3/thu

```

          29 L3
        623607 THU/RL
L4          0 L3/THU
           (L3 (L) THU/RL)

```

=> d his

(FILE 'HOME' ENTERED AT 14:06:26 ON 01 OCT 2004)

FILE 'REGISTRY' ENTERED AT 14:06:32 ON 01 OCT 2004

```

L1          STRUCTURE UPLOADED
L2          1 S L1
L3          19 S L1 FULL

```

FILE 'HCAPLUS' ENTERED AT 14:13:42 ON 01 OCT 2004

```

L4          0 S L3/THU

```

=> s l3/prop

```

          29 L3
        3203746 PREP/RL
L5          27 L3/PROP
           (L3 (L) PREP/RL)

```

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	4.72	164.97

FILE 'REGISTRY' ENTERED AT 14:15:02 ON 01 OCT 2004

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STRUCTURE FILE UPDATES: 29 SEP 2004 HIGHEST RN 754169-63-6  
DICTIONARY FILE UPDATES: 29 SEP 2004 HIGHEST RN 754169-63-6

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See [HELP CROSSOVER](#) for details.

Experimental and calculated property data are now available. For more information enter [HELP PROP](#) at an arrow prompt in the file or refer to the file summary sheet on the web at:



<http://www.cas.org/ONLINE/DBSS/registryss.html>

=> e pyridinium ion/cn

```

E1      1      PYRIDINIUM IODINE DIBROMIDE/CN
E2      1      PYRIDINIUM IODINE DICHLORIDE/CN
E3      1  --> PYRIDINIUM ION/CN
E4      1      PYRIDINIUM ION, 3-BROMO-/CN
E5      1      PYRIDINIUM ION, 4-AMINO-/CN
E6      1      PYRIDINIUM ION, 4-BROMO-/CN
E7      1      PYRIDINIUM L-ASCORBATE 2-SULFATE/CN
E8      1      PYRIDINIUM LANOSTEROL SULFATE/CN
E9      1      PYRIDINIUM M-NITROBENZENESULFONATE/CN
E10     1      PYRIDINIUM MER-TRICHLORO(1,2-NAPHTHOQUINONE 1-OXIMATO) (PYRID
            INE) IRIDATE(1-)/CN
E11     1      PYRIDINIUM MESYLATE/CN
E12     1      PYRIDINIUM METHANESULFONATE/CN

```

=> s e3

L6 1 "PYRIDINIUM ION"/CN

=> file hcaplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	4.85	169.82

FILE 'HCAPLUS' ENTERED AT 14:15:31 ON 01 OCT 2004  
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FILE COVERS 1907 - 1 Oct 2004 VOL 141 ISS 15  
 FILE LAST UPDATED: 30 Sep 2004 (20040930/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l6/rct

```

          717 L6
          2662823 RCT/RL
L7      99 L6/RCT
          (L6 (L) RCT/RL)

```

=> d his

(FILE 'HOME' ENTERED AT 14:06:26 ON 01 OCT 2004)

FILE 'REGISTRY' ENTERED AT 14:06:32 ON 01 OCT 2004

L1 STRUCTURE UPLOADED

L2 1 S L1  
L3 19 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 14:13:42 ON 01 OCT 2004

L4 0 S L3/THU  
L5 27 S L3/PREP

FILE 'REGISTRY' ENTERED AT 14:15:02 ON 01 OCT 2004

E PYRIDINIUM ION/CN  
L6 1 S E3

FILE 'HCAPLUS' ENTERED AT 14:15:31 ON 01 OCT 2004

L7 99 S L6/RCT

=> s 17 and 15

L8 0 L7 AND L5

=> s 16

L9 717 L6

=> s 19 and 15

L10 0 L9 AND L5

=> file reg

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
2.36	172.18

FULL ESTIMATED COST

FILE 'REGISTRY' ENTERED AT 14:16:01 ON 01 OCT 2004

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STRUCTURE FILE UPDATES: 29 SEP 2004 HIGHEST RN 754169-63-6  
DICTIONARY FILE UPDATES: 29 SEP 2004 HIGHEST RN 754169-63-6

TSKA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:  
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=>

L11 STRUCTURE UPLOADED

=> s 111

SAMPLE SEARCH INITIATED 14:17:49 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 5872 TO ITERATE

17.0% PROCESSED 1000 ITERATIONS  
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

16 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
 BATCH \*\*COMPLETE\*\*  
 PROJECTED ITERATIONS: 112846 TO 122034  
 PROJECTED ANSWERS: 1298 TO 2460

L12 16 SEA SSS SAM L11

=> s l11 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS  
 DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y  
 FULL SEARCH INITIATED 14:17:55 FILE 'REGISTRY'  
 FULL SCREEN SEARCH COMPLETED - 116210 TO ITERATE

100.0% PROCESSED 116210 ITERATIONS 2489 ANSWERS  
 SEARCH TIME: 00.00.01

L13 2489 SEA SSS FUL L11

=> file hcaplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	156.26	328.44

FILE 'HCAPLUS' ENTERED AT 14:17:59 ON 01 OCT 2004  
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FILE COVERS 1907 - 1 Oct 2004 VOL 141 ISS 15  
 FILE LAST UPDATED: 30 Sep 2004 (20040930/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l13

L14 4838 L13

=> s l14 and boice, g?/au

7 BOICE, G?/AU

L15 1 L14 AND BOICE, G?/AU

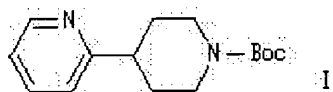
=> d l15, ibib abs fhitstr, i

L15 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2004 ACS on STN

Full  
Text

Cited  
References

ACCESSION NUMBER: 2004:511300 HCAPLUS  
 DOCUMENT NUMBER: 141:174054  
 TITLE: Direct synthesis of 4-arylpiperidines via palladium/copper(I)-cocatalyzed Negishi coupling of a 4-piperidylzinc iodide with aromatic halides and triflates  
 AUTHOR(S): Corley, Edward G.; Conrad, Karen; Murry, Jerry A.; Savarin, Cecile; Holko, Justin; **Boice, Genevieve**  
 CORPORATE SOURCE: Departments of Process Research, and Chemical Engineering Research & Development, Merck Research Laboratories, Merck and Co., Inc., Rahway, NJ, 07065, USA  
 SOURCE: Journal of Organic Chemistry (2004), 69(15), 5120-5123  
 CODEN: JOCEAH; ISSN: 0022-3263  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI



AB A general procedure for the synthesis of 4-arylpiperidines, e.g., I, via the coupling of 4-(N-Boc-piperidyl)zinc iodide with aryl halides and triflates is presented. The reaction required cocatalysis with both Cl<sub>2</sub>Pd(dppf) and a copper(I) species. An improved, safer procedure for the activation of zinc dust is also presented.

IT 57381-37-0, 2-Bromo-5-chlorobenzonitrile

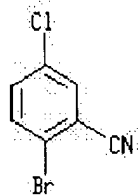
RL: RCT (Reactant); RACT (Reactant or reagent)

(prepn. of N-(Boc)-arylpiperidines via addn. of zinc to

N-(Boc)-iodopiperidine followed by palladium/copper-catalyzed Negishi coupling with aryl halides and triflates)

RN 57381-37-0 HCAPLUS

CN Benzonitrile, 2-bromo-5-chloro- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d his

(FILE 'HOME' ENTERED AT 14:06:26 ON 01 OCT 2004)

FILE 'REGISTRY' ENTERED AT 14:06:32 ON 01 OCT 2004

L1 STRUCTURE UPLOADED

L2 1 S L1

L3 19 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 14:13:42 ON 01 OCT 2004

L4 0 S L3/THU  
L5 27 S L3/PREP

FILE 'REGISTRY' ENTERED AT 14:15:02 ON 01 OCT 2004  
E PYRIDINIUM ION/CN

L6 1 S E3

FILE 'HCAPLUS' ENTERED AT 14:15:31 ON 01 OCT 2004

L7 99 S L6/RCT  
L8 0 S L7 AND L5  
L9 717 S L6  
L10 0 S L9 AND L5

FILE 'REGISTRY' ENTERED AT 14:16:01 ON 01 OCT 2004

L11 STRUCTURE UPLOADED  
L12 16 S L11  
L13 2489 S L11 FULL

FILE 'HCAPLUS' ENTERED AT 14:17:59 ON 01 OCT 2004

L14 4838 S L13  
L15 1 S L14 AND BOICE, G?/AU

=> s l14 not l15

L16 4837 L14 NOT L15

=> s l16 and conrad, k?/au

219 CONRAD, K?/AU  
L17 0 L16 AND CONRAD, K?/AU

=> s l16 and corley, e?/au

59 CORLEY, E?/AU  
L18 0 L16 AND CORLEY, E?/AU

=> s l16 and matty, l?/au

16 MATTY, L?/AU  
L19 0 L16 AND MATTY, L?/AU

=> s l16 and murray, j?/au

60 MURRY, J?/AU  
L20 0 L16 AND MURRY, J?/AU

=> s l16 and savarin, c?/au

14 SAVARIN, C?/AU  
L21 0 L16 AND SAVARIN, C?/AU

=> d his

(FILE 'HOME' ENTERED AT 14:06:26 ON 01 OCT 2004)

FILE 'REGISTRY' ENTERED AT 14:06:32 ON 01 OCT 2004

L1 STRUCTURE UPLOADED  
L2 1 S L1  
L3 19 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 14:13:42 ON 01 OCT 2004

L4 0 S L3/THU  
L5 27 S L3/PREP

FILE 'REGISTRY' ENTERED AT 14:15:02 ON 01 OCT 2004  
E PYRIDINIUM ION/CN

L6 1 S E3

FILE 'HCAPLUS' ENTERED AT 14:15:31 ON 01 OCT 2004

L7 99 S L6/RCT  
L8 0 S L7 AND L5  
L9 717 S L6  
L10 0 S L9 AND L5

FILE 'REGISTRY' ENTERED AT 14:16:01 ON 01 OCT 2004

L11 STRUCTURE UPLOADED  
L12 16 S L11  
L13 2489 S L11 FULL

FILE 'HCAPLUS' ENTERED AT 14:17:59 ON 01 OCT 2004

L14 4838 S L13  
L15 1 S L14 AND BOICE, G?/AU  
L16 4837 S L14 NOT L15  
L17 0 S L16 AND CONRAD, K?/AU  
L18 0 S L16 AND CORLEY, E?/AU  
L19 0 S L16 AND MATTY, L?/AU  
L20 0 S L16 AND MURRY, J?/AU  
L21 0 S L16 AND SAVARIN, C?/AU

=> d 116, ibib abs fhitrstr, 1-10

L16 ANSWER 1 OF 4837 HCAPLUS COPYRIGHT 2004 ACS on STN

Full  
Text

Citing  
References

ACCESSION NUMBER: 2004:779171 HCAPLUS  
TITLE: Indoor air conditioning system containing sustained-release antimicrobial element  
INVENTOR(S): Sunagawa, Minoru; Kudo, Toshihiko; Matsuoka, Masayuki  
PATENT ASSIGNEE(S): Toshiba Carrier Co., Ltd., Japan; Kodech Chemical K. K.  
SOURCE: Jpn. Kokai Tokkyo Koho, 9 pp.  
CODEN: JKXXAF  
DOCUMENT TYPE: Patent  
LANGUAGE: Japanese  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2004263917	A2	20040924	JP 2003-53436	20030228
PRIORITY APPLN. INFO.:			JP 2003-53436	20030228

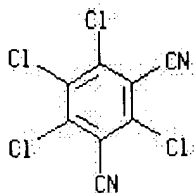
AB The invention relates to an indoor air conditioning system characterized by including solid antibacterial/antifungal element contg. I2-encapsulated microcapsules and gum rosin, wherein the system shows sustained antimicrobial effect. An indoor air conditioning system having a nonwoven fabric pouch contg. antibacterial/antifungal agent powder with resin and/or wax is also disclosed. A solid antibacterial/antifungal element was prepd. from hydrogenated terpene, dimethylsulfoxide, esterified gum rosin, and I2-encapsulated cyclodextrin for use in an indoor air conditioning system.

IT INDEXING IN PROGRESS

IT 1897-45-6, 2,4,5,6-Tetrachloroisophthalonitrile

RL: BUU (Biological use, unclassified); DEV (Device component use); THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
(indoor air conditioning system contg. sustained-release antimicrobial element with resin and/or wax)

RN 1897-45-6 HCAPLUS  
 CN 1,3-Benzenedicarbonitrile, 2,4,5,6-tetrachloro- (9CI) (CA INDEX NAME)



L16 ANSWER 2 OF 4837 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text Citing References

ACCESSION NUMBER: 2004:753382 HCAPLUS  
 TITLE: Preparation of (perfluoroalkyl)benzonitriles  
 INVENTOR(S): Okumura, Yasunori; Masuda, Takeshi; Nishimae, Shinji; Asako, Yoshinobu  
 PATENT ASSIGNEE(S): Nippon Shokubai Co., Ltd., Japan  
 SOURCE: Jpn. Kokai Tokkyo Koho, 15 pp.  
 CODEN: JKXXAF  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2004256399	A2	20040916	JP 2003-46101	20030224
PRIORITY APPLN. INFO.:			JP 2003-46101	20030224

AB Title compds. I (R1 = perfluoroalkyl; a = 1, 2; b = 1-4; c = 0-4; d = 0-2; a + b + c + d = 6), useful as intermediates for dyes, pharmaceuticals, agrochems., polymers, etc., are prepd. by reaction of tetrafluorophthalonitrile (II) with R2Si(R3)3 (R2 = perfluoroalkyl; R3 = alkyl). II was treated with F3CSiMe3 in N-methylpyrrolidinone-DMF in the presence of CuI and KF at 50° for 8 h to give 9% 3-amino-6-fluoro-4,5-bis(trifluoromethyl)phthalonitrile and 3% 2-amino-5-fluoro-3,4,6-tris(trifluoromethyl)benzonitrile.

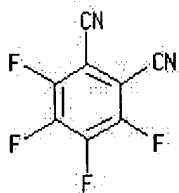
IT INDEXING IN PROGRESS

IT 1835-65-0, Tetrafluorophthalonitrile

RL: RCT (Reactant); RACT (Reactant or reagent)  
 (prepn. of (perfluoroalkyl)benzonitriles from tetrafluorophthalonitrile and perfluoroalkylsilanes)

RN 1835-65-0 HCAPLUS

CN 1,2-Benzenedicarbonitrile, 3,4,5,6-tetrafluoro- (9CI) (CA INDEX NAME)



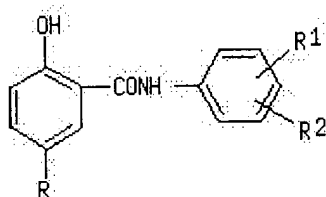
L16 ANSWER 3 OF 4837 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text Citing References

ACCESSION NUMBER: 2004:741848 HCAPLUS  
 TITLE: Low-pollution antifouling coating compositions

INVENTOR(S): Kohara, Masanori; Yoshimaru, Masaaki; Morishita, Toshio  
 PATENT ASSIGNEE(S): Api Corporation, Japan  
 SOURCE: Jpn. Kokai Tokkyo Koho, 17 pp.  
 CODEN: JKXXAF  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2004250653	A2	20040909	JP 2003-92701	20030221
PRIORITY APPLN. INFO.: GI			JP 2003-92701	20030221



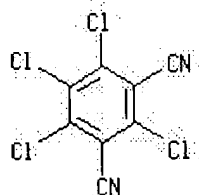
AB The coating comps. contain (a) I (R = C1-8 alkyl; R1, R2 = H, C1-4 alkyl, NO2, where R1 and R2 are not H simultaneously) such as 5-tert-butyl-2'-methyl-4'-nitrosalicylanilide, (b) silicone oil, (c) hydrolyzable polymers, and (d) elution control agents such as dialkyl polysulfides and polybutene. The coatings are useful for fish nets, ships, ropes, etc.

IT **1897-45-6**, 1,3-Dicyanotetrachlorobenzene

RL: TEM (Technical or engineered material use); USES (Uses)  
 (low-pollution antifouling coating comps. contg. salicylanilides)

RN **1897-45-6** HCAPLUS

CN 1,3-Benzenedicarbonitrile, 2,4,5,6-tetrachloro- (9CI) (CA INDEX NAME)



L16 ANSWER 4 OF 4837 HCAPLUS COPYRIGHT 2004 ACS on STN

Full  
Text

Chemical  
References

ACCESSION NUMBER:

2004:740130 HCAPLUS

TITLE:

Preparation of pyrazolopurine-based tricyclic compounds for the treatment of inflammatory and immune diseases

INVENTOR(S):

Qiu, Yuping; Belema, Makonen; Yang, Xuejie; Zusi, Fred Christopher; Pitts, William J.

PATENT ASSIGNEE(S):

Bristol-Myers Squibb Company, USA

SOURCE:

PCT Int. Appl., 127 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English



FAMILY ACC. NUM. COUNT: 1

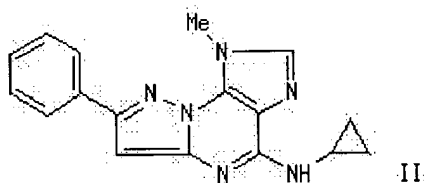
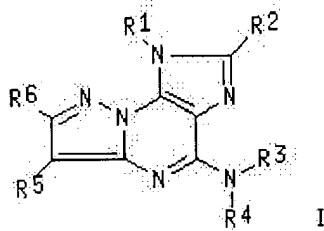
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004075846	A2	20040910	WO 2004-US5384	20040224
W: AE, AE, AG, AL, AL, AM, AM, AM, AT, AT, AU, AZ, AZ, BA, BB, BG, BG, BR, BR, BW, BY, BY, BZ, BZ, CA, CH, CN, CN, CO, CO, CR, CR, CU, CU, CZ, CZ, DE, DE, DK, DK, DM, DZ, EC, EC, EE, EE, EG, ES, ES, FI, FI, GB, GD, GE, GE, GH, GM, HR, HR, HU, HU, ID, IL, IN, IS, JP, JP, KE, KE, KG, KG, KP, KP, KR, KR, KZ, KZ, KZ, LC, LK, LR, LS, LS, LT, LU, LV, MA, MD, MD, MG, MK, MN, MW, MX, MX, MZ, MZ, NA, NI RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				

PRIORITY APPLN. INFO.:US 2003-449770P

P 20030225

GI



AB The title compds. I [R1 = H, alkyl, alkenyl, alkynyl, haloalkyl, etc.; R2 = H, halo, CN, alkyl, alkenyl, alkynyl, etc.; R3, R4 = H, alkyl, alkenyl, alkynyl, haloalkyl, etc., or R3R4 together with the nitrogen atom to which they are attached to form a heterocycle; R5 = H, OH, halo, CN, alkyl, alkenyl, alkynyl, etc.] were prepd. for the treatment of inflammatory and immune diseases. For example, reaction of 1-methyl-7-phenyl-4H-pyrazolo[5,1b]purin-4-one (prepn. given) with cyclopropylamine yielded compd. II. The compds. of this invention are active in vitro in the LPS-induced TNF $\alpha$  secretion model.

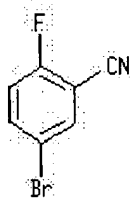
IT 179897-89-3

RL: RCT (Reactant); RACT (Reactant or reagent)

(prepn. of pyrazolopurine-based tricyclic compds. for the treatment of inflammatory and immune diseases)

RN 179897-89-3 HCAPLUS

CN Benzonitrile, 5-bromo-2-fluoro- (9CI) (CA INDEX NAME)



L16 ANSWER 5 OF 4837 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text	Citing References
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ACCESSION NUMBER: 2004:725629 HCAPLUS  
 DOCUMENT NUMBER: 141:201726  
 TITLE: Technology for cultivation of Taishan Polygonum multiflorum  
 INVENTOR(S): Zhang, Yuqing  
 PATENT ASSIGNEE(S): Peop. Rep. China  
 SOURCE: Faming Zhuanli Shenqing Gongkai Shuomingshu, 7 pp.  
 CODEN: CNXXEV  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Chinese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CN 1408204	A	20030409	CN 2002-130717	20020918
			CN 2002-130717	20020918

## PRIORITY APPLN. INFO.:

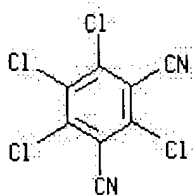
AB The title technol. comprises the following steps of (1) making pH=6-7 soil into ridge, sterilizing with phoxim and chlorothalonil, flatting soil, watering, sowing 10-15 g/m<sup>2</sup> seed, and covering with 2-3 cm thickness soil; (2) spraying seedlings with 1:500 aq. chlorothalonil soln. for 1-3 times, cultivating till the seedlings have 2-4 leaves; (3) harrowing pH=6-7 soil, applying 3,000-7,000 kg farm manure, ridging, dibbling every 7-10 cm, planting the seedlings, watering, and sealing the holes; setting shelves with height 1.5-2.0 m, and keeping the relative moisture 50-95%.; and (5) picking the seeds, drying, excavating the root tuber at below 10° in the autumn, and packing. The seeds should be sterilized by immersing into aq. carbendazim or chlorothalonil soln. for 20-24 h.

IT 1897-45-6, Chlorothalonil

RL: AGR (Agricultural use); BIOL (Biological study); USES (Uses)  
 (technol. for cultivation of Taishan Polygonum multiflorum)

RN 1897-45-6 HCAPLUS

CN 1,3-Benzenedicarbonitrile, 2,4,5,6-tetrachloro- (9CI) (CA INDEX NAME)



L16 ANSWER 6 OF 4837 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text	Citing References
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ACCESSION NUMBER: 2004:719892 HCAPLUS  
 DOCUMENT NUMBER: 141:243559  
 TITLE: Preparation of 3-phenyl-6-(trifluoromethyl)uracils as insecticides

INVENTOR(S): Schwarz, Hans-Georg; Andree, Roland; Hoischen, Dorothee; Linker, Karl-Heinz; Kluth, Joachim; Schallner, Otto; Drewes, Mark Wilhelm; Dahmen, Peter; Feucht, Dieter; Pontzen, Rolf; Loesel, Peter; Auler, Thomas; Hills, Martin; Kehne, Heinz

PATENT ASSIGNEE(S): Bayer CropScience AG, Germany

SOURCE: Ger. Offen., 51 pp.  
CODEN: GWXXBX

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

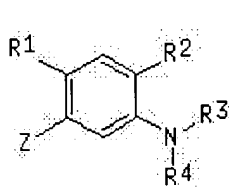
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 10307142	A1	20040902	DE 2003-10307142	20030220
WO 2004074274	A1	20040902	WO 2004-EP1198	20040210

W: AE, AE, AG, AL, AL, AM, AM, AM, AT, AT, AU, AZ, AZ, BA, BB, BG, BG, BR, BR, BW, BY, BY, BZ, BZ, CA, CH, CN, CN, CO, CO, CR, CR, CU, CU, CZ, CZ, DE, DE, DK, DK, DM, DZ, EC, EC, EE, EE, EG, ES, ES, FI, FI, GB, GD, GE, GE, GH, GM, HR, HR, HU, HU, ID, IL, IN, IS, JP, JP, KE, KE, KG, KG, KP, KP, KR, KR, KZ, KZ, KZ, LC, LK, LR, LS, LS, LT, LU, LV, MA, MD, MD, MG, MK, MN, MW, MX, MX, MZ, MZ, NA, NI

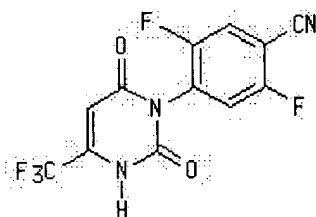
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.:  
GI

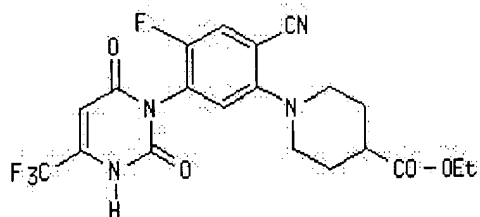
DE 2003-10307142 A 20030220



I



II



III

AB Title compds. I [R1 = H, CN, halo; R2 = NO2, CN, thiocarbamoyl; R3, R4 = together with the N-atom form a monocyclic or bicyclic ring with provisos; Z = heterocyclic ring, e.g., s-triazol-3-ols, pyrrole-2,5-diones, 2,4-dioxypyrimidines, etc.] were prepd. For example, N-alkylation of piperidine-4-carboxylic acid Et ester by difluorophenyl II, afforded trifluoromethyluracil III in 40% yield. In spider mite control assays,

3-examples of compds. I showed good effectiveness (sic).

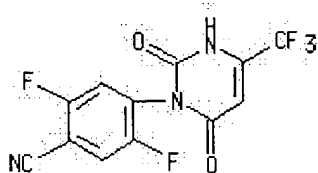
IT 162926-25-2, 3-(4-Cyano-2,5-difluorophenyl)-6-trifluoromethyl-1H-pyrimidin-2,4-dione

RL: RCT (Reactant); RACT (Reactant or reagent)

(prepn. of phenyltrifluoromethyluracils as insecticides)

RN 162926-25-2 HCAPLUS

CN Benzonitrile, 4-[3,6-dihydro-2,6-dioxo-4-(trifluoromethyl)-1(2H)-pyrimidinyl]-2,5-difluoro- (9CI) (CA INDEX NAME)

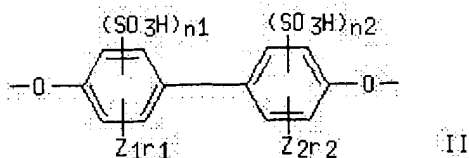
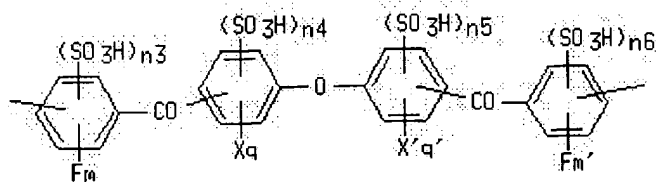


L16 ANSWER 7 OF 4837 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text      Citings  
References

ACCESSION NUMBER: 2004:700578 HCAPLUS  
DOCUMENT NUMBER: 141:210090  
TITLE: Sulfonated fluorine-containing polyaryl ethers, their compositions, moldings, and polymer electrolyte membranes  
INVENTOR(S): Sakaguchi, Yoshimitsu; Kitamura, Kota; Nagahara, Shigenori; Omote, Kazushi; Nishichi, Ai; Asako, Yoshinobu  
PATENT ASSIGNEE(S): Toyobo Co., Ltd., Japan; Nippon Shokubai Co., Ltd.  
SOURCE: Jpn. Kokai Tokkyo Koho, 35 pp.  
CODEN: JKXXAF  
DOCUMENT TYPE: Patent  
LANGUAGE: Japanese  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2004238424	A2	20040826	JP 2003-26294	20030203
PRIORITY APPLN. INFO.: GI			JP 2003-26294	20030203



AB The polyaryl ethers have repeating units of I [ $m, m' = 0-4, (m + m') = 1-8; X, X' = \text{halo}, \text{C1-6 lower alk(ox)yl}; q, q' = 0-4; n1-n6 = 0-2, (n1 + n2 + n3 + n4 + n5 + n6) = 1-12; (n3 + m) \leq 4, (n4 + q) \leq 4,$

$(n_5 + q') \leq 4$ ,  $(n_6 + m') \leq 4$ ] and II [Z1, Z2 = C1-6 lower alkyl, alkoxyl, carboxyl, carbonyl, nitro, amino, OH, halo;  $r_1, r_2 = 0-4$ ;  $(n_1 + r_1) \leq 4$ ,  $(n_2 + r_2) \leq 4$ ], and/or repeating units of III and IV [ $s = 1, 2$ ;  $n_7, n_8, n_9 = 0-2$ ,  $(n_7 + n_8 + n_9) = 1-6$ ; Z3, Z4 = C1-6 lower alkyl, alkoxyl, carboxyl, carbonyl, nitro, amino, OH, halo;  $r_3, r_4 = 0-4$ ;  $(n_7 + r_3) \leq 4$ ,  $(n_8 + r_4) \leq 4$ ]. The membranes, useful for fuel cell electrolytes, have desirable amts. of sulfonic acid groups, and show improved ionic cond. and heat resistance.

IT **744229-30-9DP**, sulfonated

RL: DEV (Device component use); IMF (Industrial manufacture); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses) (sulfonated F-contg. polyaryl ethers for polymer electrolyte membranes with good durability)

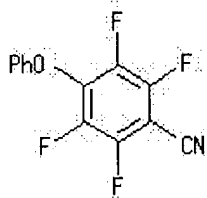
RN 744229-30-9 HCAPLUS

CN Benzonitrile, 2,3,5,6-tetrafluoro-4-phenoxy-, polymer with [1,1'-biphenyl]-4,4'-diol and 4,4'-[2,2,2-trifluoro-1-(trifluoromethyl)ethylidene]bis[phenol] (9CI) (CA INDEX NAME)

CM 1

CRN 67600-87-7

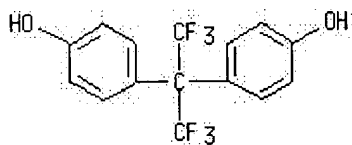
CMF C13 H5 F4 N O



CM 2

CRN 1478-61-1

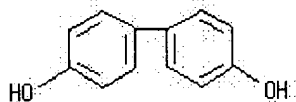
CMF C15 H10 F6 O2



CM 3

CRN 92-88-6

CMF C12 H10 O2



L16 ANSWER 8 OF 4837 HCAPLUS COPYRIGHT 2004 ACS on STN

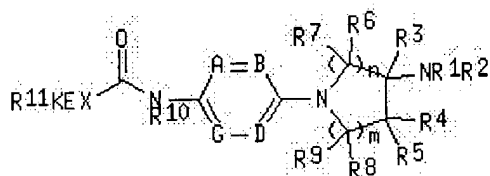
Full Text References

ACCESSION NUMBER:

2004:696342 HCAPLUS

DOCUMENT NUMBER: 141:225302  
 TITLE: Preparation of N-arylheterocycles as melanin concentrating hormone (MCH) antagonists.  
 INVENTOR(S): Schwink, Lothar; Stengelin, Siegfried; Gossel, Matthias; Boehme, Thomas; Hessler, Gerhard; Stahl, Petra; Gretzke, Dirk  
 PATENT ASSIGNEE(S): Aventis Pharma Deutschland GmbH, Germany  
 SOURCE: PCT Int. Appl., 390 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: German  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004072025	A2	20040826	WO 2004-EP1342	20040213
W: AE, AE, AG, AL, AL, AM, AM, AM, AT, AT, AU, AZ, AZ, BA, BB, BG, BG, BR, BR, BW, BY, BY, BZ, BZ, CA, CH, CN, CN, CO, CO, CR, CR, CU, CU, CZ, CZ, DE, DE, DK, DK, DM, DZ, EC, EC, EE, EE, EG, ES, ES, FI, FI, GB, GD, GE, GE, GH, GM, HR, HR, HU, HU, ID, IL, IN, IS, JP, JP, KE, KE, KG, KG, KP, KP, KR, KR, KZ, KZ, KZ, LC, LK, LR, LS, LS, LT, LU, LV, MA, MD, MD, MG, MK, MN, MW, MX, MX, MZ, MZ, NA, NI RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
DE 10306250	A1	20040909	DE 2003-10306250	20030214
PRIORITY APPLN. INFO.:			DE 2003-10306250	A 20030214
GI				



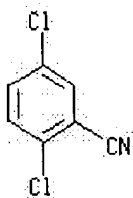
AB Title compds. [I; R1, R2 = H, alkyl, alkoxyalkyl, aryloxyalkyl, alkylcarbonyl, alkenylcarbonyl, etc.; R1R2N = atoms to form a 4-10 membered mono-, bi-, or spirocyclic (substituted) ring; R3 = H, alkyl; R4, R5 = H, alkyl, OH, alkoxy, alkylcarbonyloxy, alkylthio; R6-R9 = H, alkyl; R6R7, R8R9 = O; A, B, D, G = N, CR42; AB, DG = CR42; R42 = H, F, Cl, Br, iodo, CF3, NO2, cyano, OCF3, alkoxy, alkylthio, alkenyl, cycloalkyl, cycloalkoxy, cycloalkenyl, alkynyl, CO2H, etc.; R10 = H, alkyl, alkenyl, alkynyl; X = NR52, O, bond, C:C, C≡C, etc.; R52 = H, alkyl; E = (substituted) C3-14 carbocyclyl, heterocyclyl; K = bond, O, CH2O, S, SO, CO, C:C, C≡C, etc.; R11 = H, alkyl, alkoxyalkyl, alkenyl, alkynyl, 3-10 membered (substituted) mono-, bi-, tri- or spirocyclic ring; EKR11 = (unsatd.) tricyclic ring; m, n = 0-2], were prepd. Thus, N-[1-(4-aminophenyl)pyrrolidin-3-yl]piperidine was treated with carbonyldiimidazole and then with 4-(4-chlorophenyl)piperidine to give 4-(4-chlorophenyl)piperidine-1-carboxylic acid [4-[3-(acetylmethylamino)pyrrolidin-1-yl]phenyl]amide. The latter at 30 mg/kg orally in female NMRI mice reduced milk consumption by 64%.

IT 21663-61-6, 2,5-Dichlorobenzonitrile

RL: RCT (Reactant); RACT (Reactant or reagent)  
(prepn. of N-arylheterocycles as MCH antagonists)

RN 21663-61-6 HCAPLUS

CN Benzonitrile, 2,5-dichloro- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



L16 ANSWER 9 OF 4837 HCAPLUS COPYRIGHT 2004 ACS on STN

Full  
Text

Citing  
References

ACCESSION NUMBER:

2004:683835 HCAPLUS

TITLE:

Monitoring of pesticide residues in fresh peaches  
produced under conventional and integrated crop  
management cultivation

AUTHOR(S):

Tsakiris, I. N.; Danis, T. G.; Stratis, I. A.;  
Nikitovic, D.; Dialyna, I. A.; Alegakis, A. K.;  
Tsatsakis, A. M.

CORPORATE SOURCE:

Center of Toxicological Sciences and Research, Medical  
School, University of Crete, Crete, GR-71409, Greece

SOURCE:

Food Additives & Contaminants (2004), 21(7), 670-677  
CODEN: FACOEB; ISSN: 0265-203X

PUBLISHER:

Taylor & Francis Ltd.

DOCUMENT TYPE:

Journal

LANGUAGE:

English

AB The frequency and severity of crop protection product (pesticide) contamination of peaches grown conventionally were compared with those of peaches grown by integrated crop management (ICM). The peach samples (n = 150) were collected preharvest (June-August 2001) from both conventional (n = 55) and ICM (n = 95) cultivations from the Pella and Imathia districts of Macedonia, Northern Greece. The residue levels of selected insecticides, fungicides and acaricides in peach samples were detd. by gas chromatog.-mass spectrometry following solid-phase extn. The concns. of all detected pesticides were lower than the max. residue limits (MRLs) in all peach samples grown with the ICM system (p < 0.001). However, chlorpyrifos residues at levels higher than the MRLs were detected in four peach samples (i.e. 7% of the total samples) grown by the conventional system. Comparing the results for both cultivation methods with the reported av. percentage (3.6%) of fruit samples with pesticide residues above the MRLs (European Union report for Greece in 2001), it was concluded that the initial implementation of the ICM in Greece was successful. The present study indicates that ICM cultivation has a higher efficiency in terms of product safety and quality. Furthermore, the results suggest that the application of conventional cultivation requires continuous monitoring of various crop protection product levels.

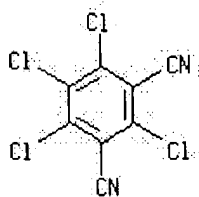
IT 1897-45-6, Chlorothalonil

RL: AGR (Agricultural use); POL (Pollutant); BIOL (Biological study); OCCU (Occurrence); USES (Uses)

(pesticide residues in fresh peaches produced under conventional and integrated crop management cultivation)

RN 1897-45-6 HCAPLUS

CN 1,3-Benzenedicarbonitrile, 2,4,5,6-tetrachloro- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 10 OF 4837 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text **Cited References**

ACCESSION NUMBER: 2004:682335 HCAPLUS  
 TITLE: Evaluation of polyaniline as a sorbent for SPE of a variety of polar pesticides from water followed by CD-MEKC-DAD  
 AUTHOR(S): Bagheri, H.; Saraji, M.; Barcelo, D.  
 CORPORATE SOURCE: Department of Chemistry, Sharif University of Technology, Tehran, Iran  
 SOURCE: Chromatographia (2004), 59(5/6), 283-289  
 CODEN: CHRGB7; ISSN: 0009-5893  
 PUBLISHER: Vieweg Verlag/GWV Fachverlage GmbH  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB A recently synthesized polyaniline (PANI) was used and evaluated as a sorbent for solid-phase extn. of a variety of polar pesticides and some of their degrdn. products from H<sub>2</sub>O samples. Several classes of pesticides including phenoxy acids, triazines, ureas, oxime carbamates and carbamates were selected for this study. The detn. of these pesticides was carried out using cyclodextrin modified micellar electrokinetic chromatog. equipped with diode array detection. The recovery results using PANI were compared with those obtained by C18, Isolute ENV+, Oasis HLB and LiChrolut EN. Effect of humic acid, as a major interference, on extn. recovery was also studied. The performance of the method was evaluated by anal. of tap and river water. The relative std. deviation of method was 6-14% (n = 3) and detection limits were at 0.01-0.5 µg L<sup>-1</sup> using 350-mL H<sub>2</sub>O samples.

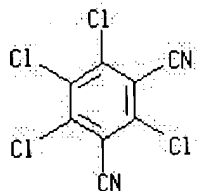
IT 1897-45-6, Chlorothalonil

RL: ANT (Analyte); ANST (Analytical study)

(evaluation of polyaniline as a sorbent for SPE of a variety of polar pesticides from water followed by CD-MEKC-DAD)

RN 1897-45-6 HCAPLUS

CN 1,3-Benzenedicarbonitrile, 2,4,5,6-tetrachloro- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d his

(FILE 'HOME' ENTERED AT 14:06:26 ON 01 OCT 2004)



FILE 'REGISTRY' ENTERED AT 14:06:32 ON 01 OCT 2004

L1 STRUCTURE UPLOADED  
L2 1 S L1  
L3 19 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 14:13:42 ON 01 OCT 2004

L4 0 S L3/THU  
L5 27 S L3/PREP

FILE 'REGISTRY' ENTERED AT 14:15:02 ON 01 OCT 2004

E PYRIDINIUM ION/CN  
L6 1 S E3

FILE 'HCAPLUS' ENTERED AT 14:15:31 ON 01 OCT 2004

L7 99 S L6/RCT  
L8 0 S L7 AND L5  
L9 717 S L6  
L10 0 S L9 AND L5

FILE 'REGISTRY' ENTERED AT 14:16:01 ON 01 OCT 2004

L11 STRUCTURE UPLOADED  
L12 16 S L11  
L13 2489 S L11 FULL

FILE 'HCAPLUS' ENTERED AT 14:17:59 ON 01 OCT 2004

L14 4838 S L13  
L15 1 S L14 AND BOICE, G?/AU  
L16 4837 S L14 NOT L15  
L17 0 S L16 AND CONRAD, K?/AU  
L18 0 S L16 AND CORLEY, E?/AU  
L19 0 S L16 AND MATTY, L?/AU  
L20 0 S L16 AND MURRY, J?/AU  
L21 0 S L16 AND SAVARIN, C?/AU

=> file reg

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	59.44	387.88
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-7.70	-7.70

FILE 'REGISTRY' ENTERED AT 14:19:45 ON 01 OCT 2004

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PLEASE SEE "[HELP USAGETERMS](#)" FOR DETAILS.

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 29 SEP 2004 HIGHEST RN 754169-63-6

DICTIONARY FILE UPDATES: 29 SEP 2004 HIGHEST RN 754169-63-6

TS/CA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See [HELP CROSSOVER](#) for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:  
<http://www.cas.org/ONLINE/DBSS/registryss.html>

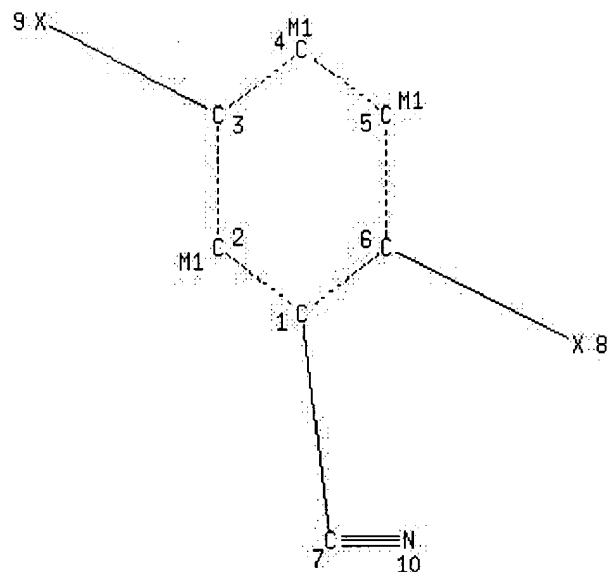
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L22 STRUCTURE UPLOADED

=> d 122

L22 HAS NO ANSWERS

L22 STR



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HCOUNT	IS M1	AT	5
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NSPEC	IS R	AT	5
NSPEC	IS R	AT	6
NSPEC	IS C	AT	7
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NSPEC	IS C	AT	9
NSPEC	IS C	AT	10

DEFAULT MLEVEL IS ATOM  
 MLEVEL IS CLASS AT 7 8 9 10  
 DEFAULT ECLEVEL IS LIMITED

# GRAPH ATTRIBUTES:

RSPEC I  
 NUMBER OF NODES IS 10

STEREO ATTRIBUTES: NONE

=> s 122

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 SAMPLE SCREEN SEARCH COMPLETED - 5872 TO ITERATE

17.0% PROCESSED 1000 ITERATIONS 0 ANSWERS  
 INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)  
 SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
 BATCH \*\*COMPLETE\*\*  
 PROJECTED ITERATIONS: 112846 TO 122034  
 PROJECTED ANSWERS: 0 TO 0

L23 0 SEA SSS SAM L22

=> s 122 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS  
 DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y  
 FULL SEARCH INITIATED 14:20:35 FILE 'REGISTRY'  
 FULL SCREEN SEARCH COMPLETED - 116210 TO ITERATE

100.0% PROCESSED 116210 ITERATIONS 24 ANSWERS  
 SEARCH TIME: 00.00.01

L24 24 SEA SSS FUL L22

=> file hcaplus

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FULL ESTIMATED COST	155.84	543.72

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	0.00	-7.70

FILE 'HCAPLUS' ENTERED AT 14:20:39 ON 01 OCT 2004  
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 PLEASE SEE "[HELP USAGETERMS](#)" FOR DETAILS.  
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FILE COVERS 1907 - 1 Oct 2004 VOL 141 ISS 15  
 FILE LAST UPDATED: 30 Sep 2004 (20040930/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 124

L25 206 L24

=> d 125, ibib abs fhitr, 1-10

L25 ANSWER 1 OF 206 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text	Citing References
--------------	----------------------

ACCESSION NUMBER:

2004:740130 HCAPLUS

TITLE:

Preparation of pyrazolopurine-based tricyclic compounds for the treatment of inflammatory and immune diseases

INVENTOR(S):

Qiu, Yuping; Belema, Makonen; Yang, Xuejie; Zusi, Fred Christopher; Pitts, William J.

PATENT ASSIGNEE(S):

Bristol-Myers Squibb Company, USA

SOURCE:

PCT Int. Appl., 127 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

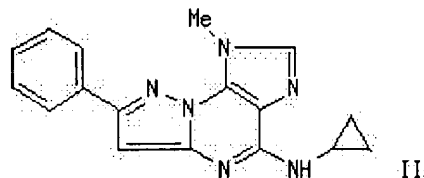
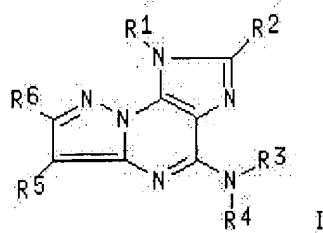
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004075846	A2	20040910	WO 2004-US5384	20040224
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RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				

PRIORITY APPLN. INFO.:

US 2003-449770P

P 20030225

GI



AB The title compds. I [R1 = H, alkyl, alkenyl, alkynyl, haloalkyl, etc.; R2 = H, halo, CN, alkyl, alkenyl, alkynyl, etc.; R3, R4 = H, alkyl, alkenyl, alkynyl, haloalkyl, etc., or R3R4 together with the nitrogen atom to which they are attached to form a heterocycle; R5 = H, OH, halo, CN, alkyl, alkenyl, alkynyl, etc.] were prepd. for the treatment of inflammatory and immune diseases. For example, reaction of 1-methyl-7-phenyl-4H-

pyrazolo[5,1b]purin-4-one (prepn. given) with cyclopropylamine yielded compd. II. The compds. of this invention are active in vitro in the LPS-induced TNF $\alpha$  secretion model.

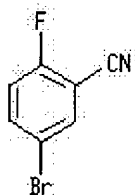
IT **179897-89-3**

RL: RCT (Reactant); RACT (Reactant or reagent)

(prepn. of pyrazolopurine-based tricyclic compds. for the treatment of inflammatory and immune diseases)

RN 179897-89-3 HCAPLUS

CN Benzonitrile, 5-bromo-2-fluoro- (9CI) (CA INDEX NAME)



L25 ANSWER 2 OF 206 HCAPLUS COPYRIGHT 2004 ACS on STN

Full  
Text

Chemical  
References

ACCESSION NUMBER: 2004:696342 HCAPLUS

DOCUMENT NUMBER: 141:225302

TITLE: Preparation of N-arylheterocycles as melanin concentrating hormone (MCH) antagonists.

INVENTOR(S): Schwink, Lothar; Stengelin, Siegfried; Gossel, Matthias; Boehme, Thomas; Hessler, Gerhard; Stahl, Petra; Gretzke, Dirk

PATENT ASSIGNEE(S): Aventis Pharma Deutschland GmbH, Germany

SOURCE: PCT Int. Appl., 390 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

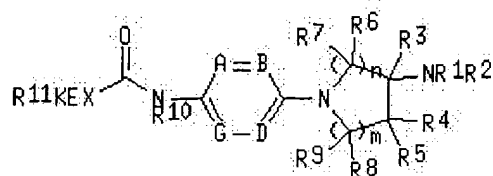
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
<u>WO 2004072025</u>	A2	20040826	<u>WO 2004-EP1342</u>	20040213
W: AE, AE, AG, AL, AL, AM, AM, AM, AT, AT, AU, AZ, AZ, BA, BB, BG, BG, BR, BR, BW, BY, BY, BZ, BZ, CA, CH, CN, CN, CO, CO, CR, CR, CU, CU, CZ, CZ, DE, DE, DK, DK, DM, DZ, EC, EC, EE, EE, EG, ES, ES, FI, FI, GB, GD, GE, GE, GH, GM, HR, HR, HU, HU, ID, IL, IN, IS, JP, JP, KE, KE, KG, KG, KP, KP, KR, KR, KZ, KZ, LC, LK, LR, LS, LS, LT, LU, LV, MA, MD, MD, MG, MK, MN, MW, MX, MX, MZ, MZ, NA, NI				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				

DE 10306250 A1 20040909 DE 2003-10306250 20030214

PRIORITY APPLN. INFO.: DE 2003-10306250 A 20030214

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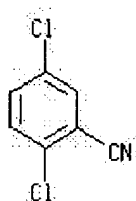
AB Title compds. [I; R1, R2 = H, alkyl, alkoxyalkyl, aryloxyalkyl, alkylcarbonyl, alkenylcarbonyl, etc.; R1R2N = atoms to form a 4-10 membered mono-, bi-, or spirocyclic (substituted) ring; R3 = H, alkyl; R4, R5 = H, alkyl, OH, alkoxy, alkylcarbonyloxy, alkylthio; R6-R9 = H, alkyl; R6R7, R8R9 = O; A, B, D, G = N, CR42; AB, DG = CR42; R42 = H, F, Cl, Br, iodo, CF3, NO2, cyano, OCF3, alkoxy, alkylthio, alkenyl, cycloalkyl, cycloalkoxy, cycloalkenyl, alkynyl, CO2H, etc.; R10 = H, alkyl, alkenyl, alkynyl; X = NR52, O, bond, C:C, C≡C, etc.; R52 = H, alkyl; E = (substituted) C3-14 carbocyclyl, heterocyclyl; K = bond, O, CH2O, S, SO, CO, C:C, C≡C, etc.; R11 = H, alkyl, alkoxyalkyl, alkenyl, alkynyl, 3-10 membered (substituted) mono-, bi-, tri- or spirocyclic ring; EKR11 = (unsatd.) tricyclic ring; m, n = 0-2], were prepd. Thus, N-[1-(4-aminophenyl)pyrrolidin-3-yl]piperidine was treated with carbonyldiimidazole and then with 4-(4-chlorophenyl)piperidine to give 4-(4-chlorophenyl)piperidine-1-carboxylic acid [4-[3-(acetylmethylamino)pyrrolidin-1-yl]phenyl]amide. The latter at 30 mg/kg orally in female NMRI mice reduced milk consumption by 64%.

IT **21663-61-6**, 2,5-Dichlorobenzonitrile

RL: RCT (Reactant); RACT (Reactant or reagent)  
(prepn. of N-arylheterocycles as MCH antagonists)

RN **21663-61-6** HCAPLUS

CN Benzonitrile, 2,5-dichloro- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



L25 ANSWER 3 OF 206 HCAPLUS COPYRIGHT 2004 ACS on STN

Full  
Text

Citing  
References

ACCESSION NUMBER: 2004:675728 HCAPLUS  
DOCUMENT NUMBER: 141:207205  
TITLE: Preparation of acrylamide derivatives as CCR antagonists  
INVENTOR(S): Shiraishi, Mitsuru; Seto, Masaki; Aikawa, Katsuji; Kanzaki, Naoyuki; Baba, Masanori  
PATENT ASSIGNEE(S): Takeda Chemical Industries, Ltd., Japan  
SOURCE: PCT Int. Appl., 284 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: Japanese  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004069808	A1	20040819	WO 2004-JP1181	20040205
W: AE, AE, AG, AL, AL, AM, AM, AM, AT, AT, AU, AZ, AZ, BA, BB, BG,				

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RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

JP 2004256530

A2

20040916

JP 2004-29681

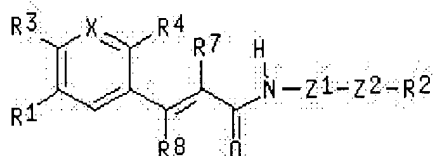
20040205

PRIORITY APPLN. INFO.:

JP 2003-31068

A 20030207

GI



AB The title compds. I [R1 represents a 5- or 6-membered ring; R3 represents hydrogen, lower alkyl, or lower alkoxy; R7 and R8 each represents hydrogen or lower alkyl; Z1 represents a 5- or 6-membered arom. ring; Z2 represents a group represented by Z2a-W1-Z2b- (Z2a and Z2b each represents oxygen, S(O)<sub>m</sub> (m is 0, 1, or 2), imino, or a bond and W1 represents an alkylene chain); X represents CR (R represents hydrogen, lower alkyl, lower alkoxy, or acyl, provided that R may form a 5- or 6-membered alicyclic heterocyclic group in cooperation with the adjacent R4) or nitrogen; R4 represents NR5R6 (R5 and R6 each represents hydrogen, a hydrocarbon group, a heterocyclic group, or acyl, or R5 is bonded to R6 to form a heterocyclic group represented by NR5R6); and R2 represents (1) amino in which the nitrogen atom may be in the form of a quaternary ammonium or oxide, (2) a nitrogenous heterocyclic group in which the ring-constituting atoms may include a sulfur or oxygen atom and the nitrogen atom may be in the form of a quaternary ammonium or oxide, etc.] are prepd. For example, (S)-(2E)-3-[4-Azepan-1-yl-4'-(2-butoxyethoxy)-1,1'-biphenyl-3-yl]-N-[4-[[[(1-propyl-1H-imidazol-5-yl)methyl]sulfinyl]phenyl]acrylamide was prepd. from (2E)-3-[4-azepan-1-yl-4'-(2-butoxyethoxy)-1,1'-biphenyl-3-yl]acrylic acid and (S)-4-[[[(1-propyl-1H-imidazol-5-yl)methyl]sulfinyl]aniline. I have excellent antagonistic activity against CCR5 and are useful as preventive/therapeutic agents for diseases caused by HIV infection in human peripheral blood mononuclear cells, esp. for AIDS. In an in vitro assay for CCR5 antagonism, compds. of this invention at 1  $\mu$ M gave 89% to 100% CCR5 binding inhibition. Formulations are given.

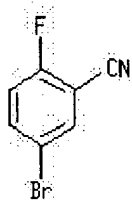
IT 179897-89-3, 5-Bromo-2-fluorobenzonitrile

RL: RCT (Reactant); RACT (Reactant or reagent)

(prepn. of acrylamide derivs. as CCR antagonists)

RN 179897-89-3 HCAPLUS

CN Benzonitrile, 5-bromo-2-fluoro- (9CI) (CA INDEX NAME)



L25 ANSWER 4 OF 206 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text	Chemical References
--------------	------------------------

ACCESSION NUMBER: 2004:648523 HCAPLUS  
 DOCUMENT NUMBER: 141:190682  
 TITLE: Preparation of indole-derived modulators of steroid hormone nuclear receptors  
 INVENTOR(S): Bell, Michael Gregory; Gavardinas, Konstantinos; Gernert, Douglas Linn; Grese, Timothy Alan; Jadhav, Prabhakar Kondaji; Lander, Peter Ambrose; Steinberg, Mitchell Irvin  
 PATENT ASSIGNEE(S): Eli Lilly and Company, USA  
 SOURCE: PCT Int. Appl., 243 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004067529	A1	20040812	WO 2004-US17	20040120
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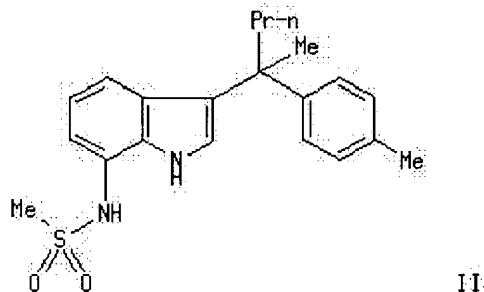
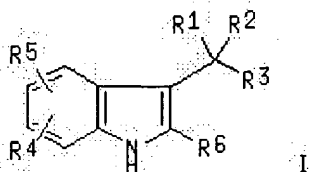
PRIORITY APPLN. INFO.:

US 2003-441947P

P 20030122

GI





AB Title compds. I [R1 = cycloalkyl, alkynyl, aryl, etc.; R2 = alkyl, cycloalkyl, aryl, etc.; R3 = alkyl, haloalkyl, cycloalkyl, etc.; R4 = H, halo, OH, amino, etc.; R5 = H, halo, OH, amino, etc.; R6 = H, halo, alkyl, etc.] are prepd. For instance, N-(1H-indol-7-yl)methanesulfonamide is reacted with the appropriate carbinol (CH<sub>2</sub>Cl<sub>2</sub>, TFA) to give II. II has K<sub>i</sub> < 500 nM for the mineralocorticoid and glucocorticoid receptor. I are useful for treating, e.g., congestive heart disease.

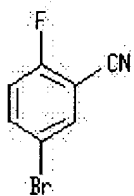
IT 179897-89-3, 5-Bromo-2-fluorobenzonitrile

RL: RCT (Reactant); RACT (Reactant or reagent)

(indole-deriv. modulators of steroid hormone nuclear receptors)

RN 179897-89-3 HCAPLUS

CN Benzonitrile, 5-bromo-2-fluoro- (9CI) (CA INDEX NAME)



L25 ANSWER 5 OF 206 HCAPLUS COPYRIGHT 2004 ACS on STN

Full  
Text

Citing  
References

ACCESSION NUMBER:

2004:550742 HCAPLUS

DOCUMENT NUMBER:

141:106471

TITLE:

Preparation of imidazo[4,5-c]pyridin-4-ones as GABA<sub>A</sub> receptor ligands for the treatment of anxiety, convulsions and cognitive disorders.

INVENTOR(S):

Goodacre, Simon Charles

PATENT ASSIGNEE(S):

UK

SOURCE:

U.S. Pat. Appl. Publ., 14 pp.

CODEN: USXXCO

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.

KIND

DATE

APPLICATION NO.

DATE

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US 2004132767	A1	20040708	US 2003-697210
PRIORITY APPLN. INFO.:			20031030
OTHER SOURCE(S):	MARPAT 141:106471		GB 2002-25399
GI			A 20021031

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB Title compds. I [X1 = H, halo, alkyl, etc.; X2 = H, halo; Y = bond, O, NH; Z = (un)substituted aryl, heteroaryl; R1 = hydrocarbon, heterocyclic, CF3C, etc.] and their pharmaceutically acceptable salts were prepd. For example, coupling of 3-fluoro-5-(4,4,5,5-tetramethyl-[1,3,2]dioxaborolan-2-yl)pyridine and bromophenyl II e.g., prepd. from 5-fluoropyridin-3-ol in 4-steps, afforded imidazopyridinone III. In human GABAA receptor binding assays, 6-examples of compds. I exhibited Ki values for displacement of [3H]-flumazenil from the  $\alpha 2$  and/or  $\alpha 3$  and/or  $\alpha 5$  subunit of the GABAA receptor of 100 nM or less. Compds. I were claimed useful for the treatment of anxiety, convulsions and cognitive disorders.

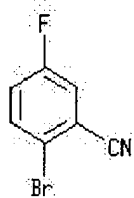
IT 57381-39-2, 2-Bromo-5-fluorobenzonitrile

RL: RCT (Reactant); RACT (Reactant or reagent)

(prepn. of imidazo[4,5-c]pyridin-4-ones as GABAA receptor ligands for the treatment of anxiety, convulsions and cognitive disorders.)

RN 57381-39-2 HCAPLUS

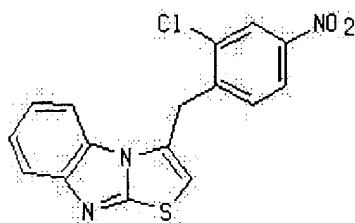
CN Benzonitrile, 2-bromo-5-fluoro- (9CI) (CA INDEX NAME)



L25 ANSWER 6 OF 206 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text	Citing References
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ACCESSION NUMBER: 2004:523233 HCAPLUS  
DOCUMENT NUMBER: 141:207126  
TITLE: Pd-Cu catalyzed heterocyclization during Sonogashira coupling: synthesis of 3-benzylthiazolo[3,2-a]benzimidazole  
AUTHOR(S): Heravi, Majid M.; Keivanloo, Ali; Rahimizadeh, Mohammad; Bakavoli, Mehdi; Ghassemzadeh, Mitra  
CORPORATE SOURCE: Department of Chemistry, School of Sciences, Azzahra University, Tehran, Iran  
SOURCE: Tetrahedron Letters (2004), 45(29), 5747-5749  
CODEN: TELEAY; ISSN: 0040-4039  
PUBLISHER: Elsevier  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI



I

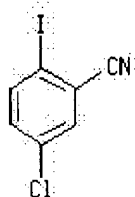
AB The reaction of 2-mercaptopropargyl benzimidazole with various iodobenzenes catalyzed by Pd-Cu leads to the formation of 3-benzylthiazolo[3,2-a]benzimidazoles, e.g., I.

IT **549547-88-8**

RL: RCT (Reactant); RACT (Reactant or reagent)  
(prepn. of benzylthiazolobenzimidazoles via palladium-copper catalyzed Sonogashira coupling of mercaptopropargyl benzimidazole with iodobenzenes followed by heterocyclization)

RN **549547-88-8** HCAPLUS

CN Benzonitrile, 5-chloro-2-iodo- (9CI) (CA INDEX NAME)



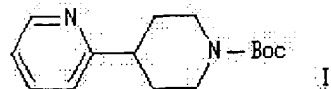
REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L25 ANSWER 7 OF 206 HCAPLUS COPYRIGHT 2004 ACS on STN

Full  
Text

Citing  
References

ACCESSION NUMBER: 2004:511300 HCAPLUS  
DOCUMENT NUMBER: 141:174054  
TITLE: Direct synthesis of 4-arylpiperidines via palladium/copper(I)-cocatalyzed Negishi coupling of a 4-piperidylzinc iodide with aromatic halides and triflates  
AUTHOR(S): Corley, Edward G.; Conrad, Karen; Murry, Jerry A.; Savarin, Cecile; Holko, Justin; Boice, Genevieve  
CORPORATE SOURCE: Departments of Process Research, and Chemical Engineering Research & Development, Merck Research Laboratories, Merck and Co., Inc., Rahway, NJ, 07065, USA  
SOURCE: Journal of Organic Chemistry (2004), 69(15), 5120-5123  
CODEN: JOCEAH; ISSN: 0022-3263  
PUBLISHER: American Chemical Society  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI



I

AB A general procedure for the synthesis of 4-arylpiperidines, e.g., I, via the coupling of 4-(N-Boc-piperidyl)zinc iodide with aryl halides and

triflates is presented. The reaction required cocatalysis with both Cl<sub>2</sub>Pd(dppf) and a copper(I) species. An improved, safer procedure for the activation of zinc dust is also presented.

IT 57381-37-0, 2-Bromo-5-chlorobenzonitrile

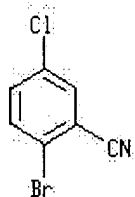
RL: RCT (Reactant); RACT (Reactant or reagent)

(prepn. of N-(Boc)-arylpiperidines via addn. of zinc to

N-(Boc)-iodopiperidine followed by palladium/copper-catalyzed Negishi coupling with aryl halides and triflates)

RN 57381-37-0 HCAPLUS

CN Benzonitrile, 2-bromo-5-chloro- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L25 ANSWER 8 OF 206 HCAPLUS COPYRIGHT 2004 ACS on STN

Full  
Text

Citing  
References

ACCESSION NUMBER: 2004:412927 HCAPLUS

DOCUMENT NUMBER: 140:423666

TITLE: A preparation of antiinflammatory 3-arylthio-3-thiazolyl-alkylamine derivatives

INVENTOR(S): Stonehouse, Jeffrey

PATENT ASSIGNEE(S): Astrazeneca AB, Swed.

SOURCE: PCT Int. Appl., 32 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

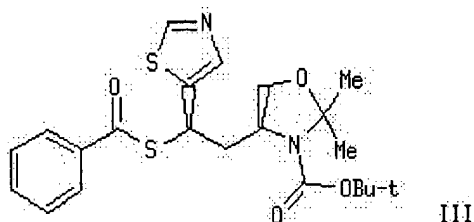
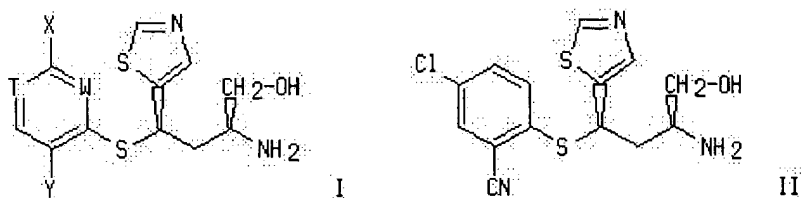
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004041794	A1	20040521	WO 2003-SE1712	20031106
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				

PRIORITY APPLN. INFO.: SE 2002-3304 A 20021107

OTHER SOURCE(S): MARPAT 140:423666

GI



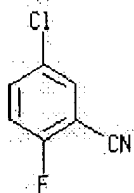
AB The invention relates to 3-arylthio-3-thiazolyl-alkylamine derivs. of formula I [wherein: T and W independently represent CR1 or N, when more than one R1 group is present, each may be selected independently; X and R1 independently represent H, Cl-4alkyl, halogen, CN, or C≡CH, etc.; Y is Cl-4alkyl, Cl-4alkoxy, halogen, CN, NO2, or CHO, etc.], useful as antiinflammatory agents. The compds. are inhibitors of nitric oxide synthase and are thereby particularly useful in the treatment or prophylaxis of inflammatory disease and pain. For instance, arylthio(thiazolyl)alkylamine deriv. II (nitric oxide synthase inhibition IC50 < 100 μM) was prepd. via reaction of thiazole deriv. III with 5-chloro-2-fluorobenzonitrile, and subsequent hydrolysis of the obtained product (example 5, no yield data).

IT **57381-34-7**, 5-Chloro-2-fluorobenzonitrile

RL: RCT (Reactant); RACT (Reactant or reagent)  
(reactant; prepn. of antiinflammatory arylthio(thiazolyl)alkylamine derivs.)

RN **57381-34-7** HCAPLUS

CN Benzonitrile, 5-chloro-2-fluoro- (9CI) (CA INDEX NAME)



L25 ANSWER 9 OF 206 HCAPLUS COPYRIGHT 2004 ACS on STN

Full  
Text

Chemical  
References

ACCESSION NUMBER:

2004:377142 HCAPLUS

DOCUMENT NUMBER:

141:123579

TITLE:

Discovery and Evaluation of Potent P1 Aryl  
Heterocycle-Based Thrombin Inhibitors

AUTHOR(S):

Young, Mary Beth; Barrow, James C.; Glass, Kristen L.;  
Lundell, George F.; Newton, Christina L.; Pellicore,  
Janetta M.; Rittle, Kenneth E.; Selnick, Harold G.;  
Stauffer, Kenneth J.; Vacca, Joseph P.; Williams,  
Peter D.; Bohn, Dennis; Clayton, Franklin C.; Cook,  
Jacquelynn J.; Krueger, Julie A.; Kuo, Lawrence C.;  
Lewis, S. Dale; Lucas, Bobby J.; McMasters, Daniel R.;

Miller-Stein, Cynthia; Pietrak, Beth L.; Wallace, Audrey A.; White, Rebecca B.; Wong, Bradley; Yan, Youwei; Nantermet, Philippe G.

CORPORATE SOURCE: Medicinal Chemistry, Pharmacology, Biological Chemistry, Structural Biology, Molecular Systems and Drug Metabolism, Merck Research Laboratories, Merck and Co. Inc., West Point, PA, 19486, USA

SOURCE: Journal of Medicinal Chemistry (2004), 47(12), 2995-3008  
CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

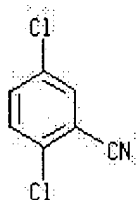
LANGUAGE: English

AB In an effort to discover potent, clin. useful thrombin inhibitors, a rapid analog synthetic approach was used to explore the P1 region. Various benzylamines were coupled to a pyridine/pyrazinone P2-P3 template. One compd., i.e. 2-[6-chloro-3-(2,2-difluoro-2-pyridin-2-yl-ethylamino)-2-oxo-2H-pyrazin-1-yl]-N-(2-[1,2,3]thiadiazol-4-yl-benzyl)acetamide, was found to have a thrombin  $K_i$  of 0.84 nM. A study of ortho-substituted five-membered-ring heterocycles was undertaken and subsequently demonstrated that the o-triazole and tetrazole rings were optimal. Combination of these potent P1 aryl heterocycles with a variety of P2-P3 groups produced a compd. with an extraordinary thrombin inhibitory activity of 1.4 pM. It is hoped that this potency enhancement in P1 will allow for more diversification in the P2-P3 region to ultimately address addnl. pharmacol. concerns.

IT 21663-61-6, 2,5-Dichlorobenzonitrile  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(prepn. of P1 aryl heterocycle-based thrombin inhibitors)

RN 21663-61-6 HCAPLUS

CN Benzonitrile, 2,5-dichloro- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L25 ANSWER 10 OF 206 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text	Cited References
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ACCESSION NUMBER: 2004:365206 HCAPLUS

DOCUMENT NUMBER: 141:88996

TITLE: A single step synthesis of 6-aminophenanthridines from anilines and 2-chlorobenzonitriles

AUTHOR(S): Gug, Fabienne; Bach, Stephane; Blondel, Marc; Vierfond, Jean-Michel; Martin, Anne-Sophie; Galons, Herve

CORPORATE SOURCE: Laboratoire de Chimie Organique, Universite Rene Descartes, Paris, 75006, Fr.

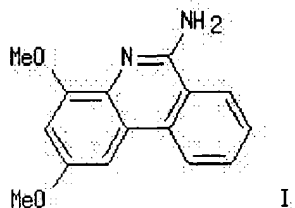
SOURCE: Tetrahedron (2004), 60(21), 4705-4708  
CODEN: TETRAB; ISSN: 0040-4020

PUBLISHER: Elsevier Science B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



AB Biol. active 6-aminophenanthridines, e.g., I, were prepd. in a single step procedure. Metal amides, in liq. ammonia, promoted the condensation of anilines with 2-chloro-benzonitriles. 6-Aminophenanthridines were isolated in moderate yield.

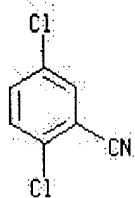
IT 21663-61-6, 2,5-Dichlorobenzonitrile

RL: RCT (Reactant); RACT (Reactant or reagent)

(prepn. of aminophenanthridines via heterocyclization of anilines with chlorobenzonitriles)

RN 21663-61-6 HCAPLUS

CN Benzonitrile, 2,5-dichloro- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> file uspatfull

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
49.96	593.68

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
-7.00	-14.70

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FILE 'USPATFULL' ENTERED AT 14:21:07 ON 01 OCT 2004

CA INDEXING COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)

FILE COVERS 1971 TO PATENT PUBLICATION DATE: 30 Sep 2004 (20040930/PD)

FILE LAST UPDATED: 30 Sep 2004 (20040930/ED)

HIGHEST GRANTED PATENT NUMBER: US6799328

HIGHEST APPLICATION PUBLICATION NUMBER: US2004194186

CA INDEXING IS CURRENT THROUGH 30 Sep 2004 (20040930/UPCA)

ISSUE CLASS FIELDS (/INCL) CURRENT THROUGH: 30 Sep 2004 (20040930/PD)

REVISED CLASS FIELDS (/NCL) LAST RELOADED: Aug 2004

USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Aug 2004

>>> USPAT2 is now available. USPATFULL contains full text of the	<<<
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>>> applications. USPAT2 contains full text of the latest US	<<<
>>> publications, starting in 2001, for the inventions covered in	<<<
>>> USPATFULL. A USPATFULL record contains not only the original	<<<

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>>> published document but also a list of any subsequent      <<<
>>> publications. The publication number, patent kind code, and <<<
>>> publication date for all the US publications for an invention <<<
>>> are displayed in the PI (Patent Information) field of USPATFULL <<<
>>> records and may be searched in standard search fields, e.g., /PN, <<<
>>> /PK, etc. <<<
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>>> USPATFULL and USPAT2 can be accessed and searched together <<<
>>> through the new cluster USPATALL. Type FILE USPATALL to <<<
>>> enter this cluster. <<<
>>> <<<
>>> Use USPATALL when searching terms such as patent assignees, <<<
>>> classifications, or claims, that may potentially change from <<<
>>> the earliest to the latest publication. <<<
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This file contains CAS Registry Numbers for easy and accurate substance identification.

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L3      19 S L1 FULL
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L5      27 S L3/PREP
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L6      1 S E3
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L8      0 S L7 AND L5
L9      717 S L6
L10     0 S L9 AND L5
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L13     2489 S L11 FULL
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FILE 'HCAPLUS' ENTERED AT 14:17:59 ON 01 OCT 2004

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L19     0 S L16 AND MATTY, L?/AU
L20     0 S L16 AND MURRY, J?/AU
L21     0 S L16 AND SAVARIN, C?/AU
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L23     0 S L22
L24     24 S L22 FULL
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FILE 'HCAPLUS' ENTERED AT 14:20:39 ON 01 OCT 2004

L25 206 S L24

FILE 'USPATFULL' ENTERED AT 14:21:07 ON 01 OCT 2004

=> s 124

L26 99 L24

=> s 126 and pd < april 2003

3433506 PD < APRIL 2003

(PD<20030400)

L27 63 L26 AND PD < APRIL 2003

=> d 127, ibib abs fhistr, 1-5

L27 ANSWER 1 OF 63 USPATFULL on STN

Full  
Text

CHINESE  
References

ACCESSION NUMBER: 2004:46802 USPATFULL  
TITLE: Treatment of asthma with MEK inhibitors  
INVENTOR(S): Bridges, Alexander James, Saline, MI, United States  
Dudley, David Thomas, Ann Arbor, MI, United States  
Mobley, James Leslie, Brighton, MI, United States  
Saltiel, Alan Robert, Ann Arbor, MI, United States  
PATENT ASSIGNEE(S): Warner-Lambert Company, Morris Plains, NJ, United States (U.S. corporation)

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 6696440	B1	20040224
	WO 2000040235		20000713
APPLICATION INFO.:	US 2001-889091		20010711 (9)
	WO 1999-US30419		19991221

	NUMBER	DATE
PRIORITY INFORMATION:	US 1999-115086P	19990107 (60)
DOCUMENT TYPE:	Utility	
FILE SEGMENT:	GRANTED	
PRIMARY EXAMINER:	Spivack, Phyllis G.	
ASSISTANT EXAMINER:	Delacroix-Muirheid, C.	
LEGAL REPRESENTATIVE:	Shen, Evelyn D., Harvey, Suzanne M.	
NUMBER OF CLAIMS:	13	
EXEMPLARY CLAIM:	1	
NUMBER OF DRAWINGS:	0 Drawing Figure(s); 0 Drawing Page(s)	
LINE COUNT:	2500	

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

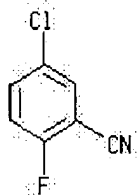
AB This invention provides a method of preventing or treating asthma by administering to a patient in need of treatment an effective amount of a selective MEK inhibitor, especially a phenyl amine of Formula I and II:  
##STR1##

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 57381-34-7P, 5-Chloro-2-fluorobenzonitrile  
(prepn. of 2-(4-bromo or 4-iodo phenylamino)benzoic acid derivs. as MEK inhibitors by addn. of halobenzoic acids to haloanilines and optional redn. or amidation of the acid)

RN 57381-34-7 USPATFULL

CN Benzonitrile, 5-chloro-2-fluoro- (9CI) (CA INDEX NAME)



L27 ANSWER 2 OF 63 USPATFULL on STN

Full Text	Chemical References
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ACCESSION NUMBER: 2003:79134 USPATFULL  
 TITLE: 2,7-substituted octahydro-1H-pyrido[1,2-A]pyrazine derivatives as ligands for serotonin receptors  
 INVENTOR(S): Desai, Kishor A., Ledyard, CT, UNITED STATES  
 Fliri, Anton F., Stonington, CT, UNITED STATES  
 Sanner, Mark A., Old Saybrook, CT, UNITED STATES  
 PATENT ASSIGNEE(S): Pfizer Inc. (U.S. corporation)

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 2003055061	A1	20030320 <--
APPLICATION INFO.:	US 2002-213604	A1	20020807 (10)
RELATED APPLN. INFO.:	Continuation of Ser. No. US 2001-784567, filed on 15 Feb 2001, ABANDONED Continuation of Ser. No. US 1999-368984, filed on 5 Aug 1999, GRANTED, Pat. No. US 6231833 Continuation-in-part of Ser. No. US 1998-135946, filed on 18 Aug 1998, ABANDONED Continuation-in-part of Ser. No. US 1997-809145, filed on 26 Mar 1997, GRANTED, Pat. No. US 5852031 A 371 of International Ser. No. WO 1995-IB689, filed on 24 Aug 1995, UNKNOWN Continuation of Ser. No. US 1994-315470, filed on 30 Sep 1994, ABANDONED		
DOCUMENT TYPE:	Utility		
FILE SEGMENT:	APPLICATION		
LEGAL REPRESENTATIVE:	PFIZER INC, 150 EAST 42ND STREET, 5TH FLOOR - STOP 49, NEW YORK, NY, 10017-5612		
NUMBER OF CLAIMS:	1		
EXEMPLARY CLAIM:	1		
LINE COUNT:	2406		

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

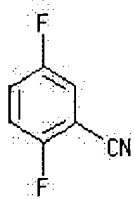
AB Substituted pyrido[1,2-a]pyrazines of general formula I; wherein Ar and Ar<sup>1</sup> represent various carbocyclic and heterocyclic aromatic rings; A represents O, S, SO, SO<sub>2</sub>, CHOH, C.dbd.O, or --(CR<sup>3R4</sup>); and n is 0-2, as well as precursors thereto, are ligands for dopamine receptor subtypes and serotonin (5HT) within the body and are therefore useful in the treatment of disorders of the dopamine and serotonin systems: ##STR1##

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 64248-64-2, 2,5-Difluorobenzonitrile  
 (prepn. of N-aryloctahydro-1H-pyrido[1,2-a]pyrazines as dopamine receptor ligands)

RN 64248-64-2 USPATFULL

CN Benzonitrile, 2,5-difluoro- (9CI) (CA INDEX NAME)



L27 ANSWER 3 OF 63 USPATFULL on STN

Full Text	Citing References
-----------	-------------------

ACCESSION NUMBER: 2003:79133 USPATFULL

TITLE: Imidazo-triazine derivatives as ligands for GABA receptors

INVENTOR(S): Carling, William Robert, Bishops Stortford, UNITED KINGDOM  
 Hallett, David James, Watford, UNITED KINGDOM  
 Russell, Michael Geoffrey Neil, Welwyn Garden City, UNITED KINGDOM  
 Street, Leslie Joseph, Little Hallingbury, UNITED KINGDOM

	NUMBER	KIND	DATE	
PATENT INFORMATION:	US 2003055060	A1	20030320	<--
	US 6617326	B2	20030909	
APPLICATION INFO.:	US 2002-195274	A1	20020715	(10)

	NUMBER	DATE
PRIORITY INFORMATION:	GB 2001-17277	20010716
DOCUMENT TYPE:	Utility	
FILE SEGMENT:	APPLICATION	
LEGAL REPRESENTATIVE:	MERCK AND CO INC, P O BOX 2000, RAHWAY, NJ, 070650907	
NUMBER OF CLAIMS:	10	
EXEMPLARY CLAIM:	1	
LINE COUNT:	1172	

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

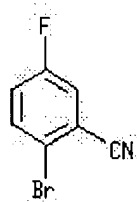
AB A class of 7-phenylimidazo[1,2-b][1,2,4]triazine derivatives, substituted at the meta position of the phenyl ring by a (cyano)(fluoro)phenyl moiety, being selective ligands for GABA<sub>A</sub> receptors, in particular having good affinity for the  $\alpha 2$  and/or  $\alpha 3$  subunit thereof, are accordingly of benefit in the treatment and/or prevention of adverse conditions of the central nervous system, including anxiety and convulsions.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 57381-39-2, 2-Bromo-5-fluorobenzonitrile  
 (prepn. of imidazo-triazines as ligands for GABA receptors)

RN 57381-39-2 USPATFULL

CN Benzonitrile, 2-bromo-5-fluoro- (9CI) (CA INDEX NAME)



L27 ANSWER 4 OF 63 USPATFULL on STN

Full Text	Ching References
--------------	---------------------

ACCESSION NUMBER: 2003:72001 USPATFULL  
 TITLE: Cyclic regimens utilizing indoline derivatives  
 INVENTOR(S): Grubb, Gary S., Newtown Square, PA, UNITED STATES  
 Fensome, Andrew, Wayne, PA, UNITED STATES  
 Miller, Lori L., Wayne, PA, UNITED STATES  
 Ullrich, John W., Exton, PA, UNITED STATES  
 Bender, Reinhold H.W., Valley Forge, PA, UNITED STATES  
 Zhang, Puwen, Audubon, PA, UNITED STATES  
 Wrobel, Jay E., Lawrenceville, NJ, UNITED STATES  
 Edwards, James P., San Diego, CA, UNITED STATES  
 Jones, Todd K., Solana Beach, CA, UNITED STATES  
 Tegley, Christopher M., Thousand Oaks, CA, UNITED STATES  
 Zhi, Lin, San Diego, CA, UNITED STATES  
 PATENT ASSIGNEE(S): WYETH, Madison, NJ (U.S. corporation)

	NUMBER	KIND	DATE	
PATENT INFORMATION:	US 2003050288	A1	20030313	<--
	US 6544970	B2	20030408	
APPLICATION INFO.:	US 2002-153393	A1	20020522	(10)
RELATED APPLN. INFO.:	Division of Ser. No. US 2000-552358, filed on 19 Apr 2000, PENDING			

	NUMBER	DATE
PRIORITY INFORMATION:	US 1999-183052P	19990504 (60)
DOCUMENT TYPE:	Utility	
FILE SEGMENT:	APPLICATION	
LEGAL REPRESENTATIVE:	HOWSON AND HOWSON, ONE SPRING HOUSE CORPORATION CENTER, BOX 457, 321 NORRISTOWN ROAD, SPRING HOUSE, PA, 19477	
NUMBER OF CLAIMS:	25	
EXEMPLARY CLAIM:	1	
LINE COUNT:	4003	

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB This invention relates to cyclic combination therapies and regimens utilizing substituted indoline derivative compounds which are antagonists of the progesterone receptor having the general structure:  
 ##STR1##

wherein R<sub>1</sub> and R<sub>2</sub> may be single substituents or fused to form spirocyclic rings, in combination with progestins, estrogens, or both. These methods of treatment may be used for contraception, for the treatment and/or prevention of secondary amenorrhea, dysfunctional bleeding, uterine leiomyomata, endometriosis, polycystic ovary syndrome, carcinomas and adenocarcinomas of the endometrium, ovary, breast, colon, or prostate, minimization of side effects, cyclic menstrual bleeding, or stimulation of food intake.

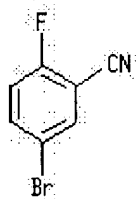
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 179897-89-3

(prepn. of oxospiro[cycloalkane-1,3'-indoline] derivs. and analogs as progesterone receptor antagonists)

RN 179897-89-3 USPATFULL

CN Benzonitrile, 5-bromo-2-fluoro- (9CI) (CA INDEX NAME)



L27 ANSWER 5 OF 63 USPATFULL on STN

Full Text	Citing References
--------------	----------------------

ACCESSION NUMBER: 2003:65387 USPATFULL

TITLE: Combination regimens using progesterone receptor modulators

INVENTOR(S): Grubb, Gary S., Newtown Square, PA, UNITED STATES  
 Zhang, Puwen, Audubon, PA, UNITED STATES  
 Terefenko, Eugene A., Quakertown, PA, UNITED STATES  
 Fensome, Andrew, Wayne, PA, UNITED STATES  
 Wrobel, Jay E., Lawrenceville, NJ, UNITED STATES  
 Fletcher, Horace, III, Pottstown, PA, UNITED STATES  
 Edwards, James P., San Diego, CA, UNITED STATES  
 Jones, Todd K., Solana Beach, CA, UNITED STATES  
 Tegley, Christopher M., Thousand Oaks, CA, UNITED STATES  
 Zhi, Lin, San Diego, CA, UNITED STATES

PATENT ASSIGNEE(S): WYETH, Madison, NJ (U.S. corporation)

	NUMBER	KIND	DATE	
PATENT INFORMATION:	<u>US 2003045511</u>	A1	20030306	<--
	<u>US 6759408</u>	B2	20040706	
APPLICATION INFO.:	<u>US 2002-141792</u>	A1	20020509	(10)
RELATED APPLN. INFO.:	Division of Ser. No. <u>US 2000-552350</u> , filed on 19 Apr 2000, PENDING			

	NUMBER	DATE
PRIORITY INFORMATION:	<u>US 1999-229346P</u>	19990504 (60)
DOCUMENT TYPE:	Utility	
FILE SEGMENT:	APPLICATION	
LEGAL REPRESENTATIVE:	HOWSON AND HOWSON, ONE SPRING HOUSE CORPORATION CENTER, BOX 457, 321 NORRISTOWN ROAD, SPRING HOUSE, PA, 19477	
NUMBER OF CLAIMS:	29	
EXEMPLARY CLAIM:	1	
LINE COUNT:	4295	

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB This invention relates to cyclic combination therapies and regimens utilizing substituted indoline derivative compounds which are antagonists of the progesterone receptor having the general structure: ##STR1##

wherein R<sup>1</sup> and R<sup>2</sup> may be single substituents or fused; R<sup>3</sup> is H, OH, NH<sub>2</sub>, C<sub>1</sub> to C<sub>6</sub> alkyl, COR<sup>C</sup>, or optionally substituted C<sub>1</sub> to C<sub>6</sub> alkyl, C<sub>3</sub> to C<sub>6</sub> alkenyl, or alkynyl; R<sup>C</sup> is H, or optionally substituted C<sub>1</sub> to C<sub>3</sub> alkyl, aryl, C<sub>1</sub> to C<sub>3</sub> alkoxy, or C<sub>1</sub> to C<sub>3</sub> aminoalkyl; R<sup>4</sup> is H, halogen, CN, NO<sub>2</sub>, or optionally substituted C<sub>1</sub> to C<sub>6</sub> alkyl, alkynyl, C<sub>1</sub> to C<sub>6</sub>

alkoxy, amino, or C<sub>1</sub> to C<sub>6</sub> aminoalkyl; and R<sup>5</sup> is a benzene ring, a five or six membered heterocyclic ring; or pharmaceutically acceptable salt thereof. Methods of treatment include contraception, secondary amenorrhea, dysfunctional bleeding, uterine leiomyomata, endometriosis, polycystic ovary syndrome, carcinomas, adenocarcinomas minimization of side effects, or food intake stimulation.

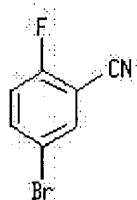
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 179897-89-3

(prepn. of substituted dihydrobenzoxazinones with progesterone receptor antagonist activity for use in contraceptive compns.)

RN 179897-89-3 USPATFULL

CN Benzonitrile, 5-bromo-2-fluoro- (9CI) (CA INDEX NAME)



=> of his

(FILE 'HOME' ENTERED AT 14:06:26 ON 01 OCT 2004)

FILE 'REGISTRY' ENTERED AT 14:06:32 ON 01 OCT 2004

L1 STRUCTURE UPLOADED  
L2 1 S L1  
L3 19 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 14:13:42 ON 01 OCT 2004

L4 0 S L3/THU  
L5 27 S L3/PREP

FILE 'REGISTRY' ENTERED AT 14:15:02 ON 01 OCT 2004  
E PYRIDINIUM ION/CN

L6 1 S E3

FILE 'HCAPLUS' ENTERED AT 14:15:31 ON 01 OCT 2004

L7 99 S L6/RCT  
L8 0 S L7 AND L5  
L9 717 S L6  
L10 0 S L9 AND L5

FILE 'REGISTRY' ENTERED AT 14:16:01 ON 01 OCT 2004

L11 STRUCTURE UPLOADED  
L12 16 S L11  
L13 2489 S L11 FULL

FILE 'HCAPLUS' ENTERED AT 14:17:59 ON 01 OCT 2004

L14 4838 S L13  
L15 1 S L14 AND BOICE, G?/AU  
L16 4837 S L14 NOT L15  
L17 0 S L16 AND CONRAD, K?/AU  
L18 0 S L16 AND CORLEY, E?/AU  
L19 0 S L16 AND MATTY, L?/AU

L20 0 S L16 AND MURRY, J?/AU  
 L21 0 S L16 AND SAVARIN, C?/AU

FILE 'REGISTRY' ENTERED AT 14:19:45 ON 01 OCT 2004

L22 STRUCTURE UPLOADED  
 L23 0 S L22  
 L24 24 S L22 FULL

FILE 'HCAPLUS' ENTERED AT 14:20:39 ON 01 OCT 2004

L25 206 S L24

FILE 'USPATFULL' ENTERED AT 14:21:07 ON 01 OCT 2004

L26 99 S L24  
 L27 63 S L26 AND PD < APRIL 2003

=> s l26 and pd < march 2003  
 3405359 PD < MARCH 2003  
 (PD<20030300)

L28 59 L26 AND PD < MARCH 2003

=> d l28, ibib abs fhitstr, 1-10

L28 ANSWER 1 OF 59 USPATFULL on STN

Full  
Text

Chgs  
References

ACCESSION NUMBER: 2004:46802 USPATFULL  
 TITLE: Treatment of asthma with MEK inhibitors  
 INVENTOR(S): Bridges, Alexander James, Saline, MI, United States  
 Dudley, David Thomas, Ann Arbor, MI, United States  
 Mobley, James Leslie, Brighton, MI, United States  
 Saltiel, Alan Robert, Ann Arbor, MI, United States  
 PATENT ASSIGNEE(S): Warner-Lambert Company, Morris Plains, NJ, United States (U.S. corporation)

	NUMBER	KIND	DATE	
PATENT INFORMATION:	US 6696440	B1	20040224	
	WO 2000040235		20000713	<--
APPLICATION INFO.:	US 2001-889091		20010711	(9)
	WO 1999-US30419		19991221	

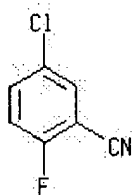
	NUMBER	DATE
PRIORITY INFORMATION:	US 1999-115086P	19990107 (60)
DOCUMENT TYPE:	Utility	
FILE SEGMENT:	GRANTED	
PRIMARY EXAMINER:	Spivack, Phyllis G.	
ASSISTANT EXAMINER:	Delacroix-Muirheid, C.	
LEGAL REPRESENTATIVE:	Shen, Evelyn D., Harvey, Suzanne M.	
NUMBER OF CLAIMS:	13	
EXEMPLARY CLAIM:	1	
NUMBER OF DRAWINGS:	0 Drawing Figure(s); 0 Drawing Page(s)	
LINE COUNT:	2500	

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB This invention provides a method of preventing or treating asthma by administering to a patient in need of treatment an effective amount of a selective MEK inhibitor, especially a phenyl amine of Formula I and II:  
 ##STR1##

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT **57381-34-7P**, 5-Chloro-2-fluorobenzonitrile  
 (prepn. of 2-(4-bromo or 4-iodo phenylamino)benzoic acid derivs. as MEK  
 inhibitors by addn. of halobenzoic acids to haloanilines and optional  
 redn. or amidation of the acid)  
 RN **57381-34-7** USPATFULL  
 CN **Benzonitrile, 5-chloro-2-fluoro- (9CI) (CA INDEX NAME)**



L28 ANSWER 2 OF 59 USPATFULL on STN

Full Text      Claim References

ACCESSION NUMBER: 2003:40676 USPATFULL  
 TITLE: 1-substituted phenyl-1-(1h-imidazol-4-yl) alcohols,  
 process for producing the same and use thereof  
 INVENTOR(S): Tasaka, Akihiro, Suita, JAPAN  
 Kaku, Tomohiro, Nishinomiya, JAPAN  
 Kusaka, Masami, Kobe, JAPAN  
 PATENT ASSIGNEE(S): Takeda Chemical Industries, Ltd., Osaka, JAPAN  
 (non-U.S. corporation)

	NUMBER	KIND	DATE	
PATENT INFORMATION:	US 6518257	B1	20030211	<--
	WO 2001030764		20010503	<--
APPLICATION INFO.:	US 2002-111136		20020418	(10)
	WO 2000-JP7284		20001019	

	NUMBER	DATE
PRIORITY INFORMATION:	JP 1999-301562	19991022
DOCUMENT TYPE:	Utility	
FILE SEGMENT:	GRANTED	
PRIMARY EXAMINER:	Stockton, Laura L.	
LEGAL REPRESENTATIVE:	Chao, Mark, Ramesh, Elaine M.	
NUMBER OF CLAIMS:	14	
EXEMPLARY CLAIM:	1	
NUMBER OF DRAWINGS:	0 Drawing Figure(s); 0 Drawing Page(s)	
LINE COUNT:	3893	

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB To provide a composition having a steroid C<sub>17</sub>,20-lyase inhibitory activity and useful as an agent for the prophylaxis or treatment of prostatism and tumors such as breast cancer. A compound represented by the formula: ##STR1##

wherein R is a hydrogen atom or a protecting group, R<sup>1</sup> is a lower alkyl group or a cyclic hydrocarbon group, R<sup>2</sup> is an aromatic hydrocarbon group optionally having substituents or an aromatic heterocyclic group optionally having substituents, R<sup>3</sup> is a hydrocarbon group optionally having substituents, a hydroxyl group optionally having substituents, a thiol group optionally having substituents, an amino group optionally having substituents, an acyl group or a halogen atom, and n is an integer of 0 to 4, and a salt



thereof have a steroid C<sub>17</sub>,20-lyase inhibitory activity, and are useful as an agent for the prophylaxis or treatment of prostatism and tumors such as breast cancer and the like.

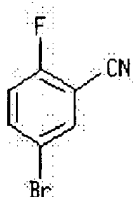
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 179897-89-3, 5-Bromo-2-fluorobenzonitrile

(prepn. process and use of phenylimidazolyl alcs. as antitumor agents)

RN 179897-89-3 USPATFULL

CN Benzonitrile, 5-bromo-2-fluoro- (9CI) (CA INDEX NAME)



L28 ANSWER 3 OF 59 USPATFULL on STN

Full  
Text

Citing  
References

ACCESSION NUMBER:

2003:20225 USPATFULL

TITLE:

Cyclocarbamate derivatives as progesterone receptor modulators

INVENTOR(S):

Zhang, Puwen, Audubon, PA, United States  
Terefenko, Eugene A., Quakertown, PA, United States  
Fensome, Andrew, Wayne, PA, United States  
Wrobel, Jay E., Lawrenceville, NJ, United States  
Fletcher, III, Horace, Pottstown, PA, United States  
Zhi, Lin, San Diego, CA, United States  
Jones, Todd K., Solana Beach, CA, United States  
Edwards, James P., San Diego, CA, United States  
Tegley, Christopher M., Thousand Oaks, CA, United States

PATENT ASSIGNEE(S):

American Home Products Corporation, Madison, NJ, United States (U.S. corporation)  
Ligand Pharmaceuticals, Inc., San Diego, CA, United States (U.S. corporation)

	NUMBER	KIND	DATE	
PATENT INFORMATION:	US 6509334	B1	20030121	<--
APPLICATION INFO.:	US 2000-552633		20000419	(9)

	NUMBER	DATE
PRIORITY INFORMATION:	US 1999-183012P	19990504 (60)
DOCUMENT TYPE:	Utility	
FILE SEGMENT:	GRANTED	
PRIMARY EXAMINER:	Ford, John M.	
LEGAL REPRESENTATIVE:	Howson and Howson	
NUMBER OF CLAIMS:	94	
EXEMPLARY CLAIM:	1	
NUMBER OF DRAWINGS:	0 Drawing Figure(s); 0 Drawing Page(s)	
LINE COUNT:	4304	

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB This invention provides compounds of Formula (I): ##STR1##

wherein R<sup>1</sup> and R<sup>2</sup> may be single substituents or fused to form

spirocyclic or hetero-spirocyclic rings;  $R^3$  is H, OH,  $NH_2$ ,  $C_1$  to  $C_6$  alkyl, substituted  $C_1$  to  $C_6$  alkyl,  $C_3$  to  $C_6$  alkenyl, substituted  $C_1$  to  $C_6$  alkenyl, alkynyl, or substituted alkynyl,  $COR^C$ ;  $R^C$  is H,  $C_1$  to  $C_3$  alkyl, substituted  $C_1$  to  $C_3$  alkyl, aryl, substituted aryl,  $C_1$  to  $C_3$  alkoxy, substituted  $C_1$  to  $C_3$  alkoxy,  $C_1$  to  $C_3$  aminoalkyl, or substituted  $C_1$  to  $C_3$  aminoalkyl;  $R^4$  is H, halogen, CN,  $NO_2$ ,  $C_1$  to  $C_6$  alkyl, substituted  $C_1$  to  $C_6$  alkyl, alkynyl, or substituted alkynyl,  $C_1$  to  $C_6$  alkoxy, substituted  $C_1$  to  $C_6$  alkoxy, amino,  $C_1$  to  $C_6$  aminoalkyl, or substituted  $C_1$  to  $C_6$  aminoalkyl; and  $R^5$  is selected from a trisubstituted benzene ring of a five or six membered ring with 1, 2, or 3 heteroatoms from the group including O, S, SO,  $SO_2$  or  $NR^6$  and containing one or two independent substituents from the group including H, halogen, CN,  $NO_2$ , amino, and  $C_1$  to  $C_3$  alkyl,  $C_1$  to  $C_3$  alkoxy,  $C_1$  to  $C_3$  aminoalkyl,  $COR^F$ , or  $NR^{G COR^F}$ ; or pharmaceutically acceptable salt thereof, as well as pharmaceutical compositions and methods using the compounds as antagonists of the progesterone receptor.

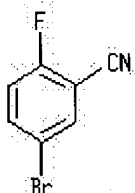
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 179897-89-3

(prepn. of benzoxazinone derivs. as progesterone receptor modulators)

RN 179897-89-3 USPATFULL

CN Benzonitrile, 5-bromo-2-fluoro- (9CI) (CA INDEX NAME)



L28 ANSWER 4 OF 59 USPATFULL on STN

Full  
Text

Claims  
References

ACCESSION NUMBER:

2002:340320 USPATFULL

TITLE:

Cyclic regimens using quinazolinone and benzoxazine derivatives

INVENTOR(S):

Grubb, Gary S., Newtown Square, PA, United States  
Zhi, Lin, San Diego, CA, United States  
Jones, Todd K., Solana Beach, CA, United States  
Zhang, Puwen, Audubon, PA, United States  
Edwards, James P., San Diego, CA, United States  
Fensome, Andrew, Wayne, PA, United States  
Terefenko, Eugene A., Quakertown, PA, United States  
Wrobel, Jay E., Lawrenceville, NJ, United States  
Tegley, Christopher M., Thousand Oaks, CA, United States

PATENT ASSIGNEE(S):

Wyeth, Madison, NJ, United States (U.S. corporation)  
Ligand Pharmaceuticals, Inc., San Diego, CA, United States (U.S. corporation)

NUMBER KIND DATE

PATENT INFORMATION: US 6498154 B1 20021224 <--  
 APPLICATION INFO.: US 2000-552357 20000419 (9)

	NUMBER	DATE
PRIORITY INFORMATION:	US 1999-183042P	19990504 (60)
DOCUMENT TYPE:	Utility	
FILE SEGMENT:	GRANTED	
PRIMARY EXAMINER:	Travers, Russell	
ASSISTANT EXAMINER:	Hui, San-ming	
LEGAL REPRESENTATIVE:	Howson and Howson	
NUMBER OF CLAIMS:	17	
EXEMPLARY CLAIM:	1	
NUMBER OF DRAWINGS:	0 Drawing Figure(s); 0 Drawing Page(s)	
LINE COUNT:	2607	

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB This invention relates to cyclic combination therapies utilizing, in combination with progestins, estrogens, or both, compounds which are progesterone receptor antagonists of the general structure: ##STR1##

wherein: R<sup>1</sup> and R<sup>2</sup> are H, COR<sup>A</sup>, or NR<sup>BCORA</sup>, alkyl, alkenyl, alkynyl, cycloalkyl, aryl, or heterocyclic; or R<sup>1</sup> and R<sup>2</sup> fuse to form 3 to 8 membered spirocyclic alkyl, alkenyl or heterocyclic rings; R<sup>A</sup> is H or optionally substituted alkyl, aryl, alkoxy, or aminoalkyl groups; R<sup>B</sup> is H or alkyl; R<sup>3</sup> is H, OH, NH<sub>2</sub>, COR<sup>C</sup> or alkyl, alkenyl, or alkynyl; R<sup>C</sup> is H, alkyl, aryl, alkoxy, or aminoalkyl; R<sup>4</sup> is H, halogen, CN, NO<sub>2</sub>, alkyl, alkynyl, alkoxy, amino or aminoalkyl; R<sup>5</sup> is benzene or 5- or 6-membered heterocyclic ring; R<sup>6</sup> is H or alkyl; G<sub>1</sub> is O, NR<sub>7</sub>, or CR<sub>7R8</sub>; G<sub>2</sub> is CO or CR<sub>7R8</sub>; provided that when G<sub>1</sub> is O, G<sub>2</sub> is CR<sub>7R8</sub>, and G<sub>1</sub> and G<sub>2</sub> cannot both be CR<sub>7R8</sub>; R<sub>7</sub> and R<sub>8</sub> are H or an optionally substituted alkyl, aryl, or heterocyclic moiety; or pharmaceutically acceptable salt thereof. These methods may be used for contraception or treatment and/or prevention of secondary amenorrhea, dysfunctional bleeding, uterine leiomyomata, endometriosis; polycystic ovary syndrome, carcinomas and adenocarcinomas of the endometrium, ovary, breast, colon, prostate, or minimization of side effects or cyclic menstrual bleeding. Additional uses of the invention include stimulation of food intake.

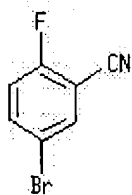
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 179897-89-3

(prepn. of substituted dihydrobenzoxazinones with progesterone receptor antagonist activity for use in contraceptive compns.)

RN 179897-89-3 USPATFULL

CN Benzonitrile, 5-bromo-2-fluoro- (9CI) (CA INDEX NAME)



L28 ANSWER 5 OF 59 USPATFULL on STN

Full Text	Citing References
--------------	----------------------

ACCESSION NUMBER: 2002:338031 USPATFULL  
 TITLE: Thrombin inhibitors  
 INVENTOR(S): Barrow, James C., Harleysville, PA, UNITED STATES  
 Coburn, Craig, Royersford, PA, UNITED STATES  
 Selnick, Harold G., Ambler, PA, UNITED STATES  
 Ngo, Phung L., Upper Darby, PA, UNITED STATES

	NUMBER	KIND	DATE	
PATENT INFORMATION:	US 2002193398	A1	20021219	<--
	US 6610701	B2	20030826	
APPLICATION INFO.:	US 2002-71422	A1	20020208	(10)

	NUMBER	DATE
PRIORITY INFORMATION:	US 2001-267960P	20010209 (60)
DOCUMENT TYPE:	Utility	
FILE SEGMENT:	APPLICATION	
LEGAL REPRESENTATIVE:	MERCK AND CO INC, P O BOX 2000, RAHWAY, NJ, 070650907	
NUMBER OF CLAIMS:	21	
EXEMPLARY CLAIM:	1	
LINE COUNT:	2878	

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

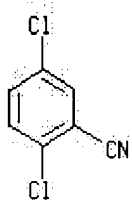
AB Compounds of the invention are useful in inhibiting thrombin and treating blood coagulation and cardiovascular disorders and have the following structure: ##STR1##

wherein

R<sup>3</sup> is hydrogen or halogen, and u is N or CH.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 21663-61-6, 2,5-Dichlorobenzonitrile  
 (prepn. of 2-(pyridin-4-yl)acetamides as thrombin inhibitors)  
 RN 21663-61-6 USPATFULL  
 CN Benzonitrile, 2,5-dichloro- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



L28 ANSWER 6 OF 59 USPATFULL on STN

Full Text	Citing References
--------------	----------------------

ACCESSION NUMBER: 2002:280635 USPATFULL  
 TITLE: Pyrazolopyrimidines as therapeutic agents  
 INVENTOR(S): Hirst, Gavin C., Marlborough, MA, UNITED STATES  
 Rafferty, Paul, Westborough, MA, UNITED STATES  
 Ritter, Kurt, Newton, GERMANY, FEDERAL REPUBLIC OF  
 Calderwood, David, Framingham, UNITED KINGDOM  
 Wishart, Neil, Jefferson, MA, UNITED STATES  
 Arnold, Lee D., Westborough, CANADA

PATENT ASSIGNEE(S): Friedman, Michael M., Newton, MA, UNITED STATES  
Abbott Laboratories, Abbott Park, IL, UNITED STATES  
(U.S. corporation)

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 2002156081	A1	20021024 <--
APPLICATION INFO.:	US 2001-815310	A1	20010322 (9)
RELATED APPLN. INFO.:	Continuation-in-part of Ser. No. US 2000-663780, filed on 15 Sep 2000, PENDING		

	NUMBER	DATE
PRIORITY INFORMATION:	US 1999-154620P	19990917 (60)
DOCUMENT TYPE:	Utility	
FILE SEGMENT:	APPLICATION	
LEGAL REPRESENTATIVE:	LAHIVE & COCKFIELD, 28 STATE STREET, BOSTON, MA, 02109	
NUMBER OF CLAIMS:	138	
EXEMPLARY CLAIM:	1	
LINE COUNT:	30126	

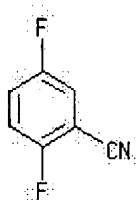
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB The present invention provides compounds of Formula I, ##STR1##

including pharmaceutically acceptable salts and/or prodrugs thereof, where G, R<sub>2</sub>, and R<sub>3</sub> are defined as described herein.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 64248-64-2, 2,5-Difluorobenzonitrile  
(prepn. of [(hetero)aryl]pyrazolo[3,4-d]pyrimidinamines as protein kinase inhibitors with antiangiogenic properties)  
RN 64248-64-2 USPATFULL  
CN Benzonitrile, 2,5-difluoro- (9CI) (CA INDEX NAME)



L28 ANSWER 7 OF 59 USPATFULL on STN

Full Text	Citing References
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ACCESSION NUMBER: 2002:262352 USPATFULL  
TITLE: Cyclic regimens utilizing indoline derivatives  
INVENTOR(S): Grubb, Gary S., Newtown Square, PA, United States  
Fensome, Andrew, Wayne, PA, United States  
Miller, Lori L., Wayne, PA, United States  
Ullrich, John W., Exton, PA, United States  
Bender, Reinhold H. W., Valley Forge, PA, United States  
Zhang, Puwen, Audubon, PA, United States  
Wrobel, Jay E., Lawrenceville, NJ, United States  
Edwards, James P., San Diego, CA, United States  
Jones, Todd K., Solana Beach, CA, United States  
Tegley, Christopher M., Thousand Oaks, CA, United States  
Zhi, Lin, San Diego, CA, United States  
PATENT ASSIGNEE(S): Wyeth, Madison, NJ, United States (U.S. corporation)

Ligand Pharmaceuticals, Inc., San Diego, CA, United States (U.S. corporation)

	NUMBER	KIND	DATE	
PATENT INFORMATION:	US 6462032	B1	20021008	<--
APPLICATION INFO.:	US 2000-552358		20000419	(9)

	NUMBER	DATE
PRIORITY INFORMATION:	US 1999-183052P	19990504 (60)
DOCUMENT TYPE:	Utility	
FILE SEGMENT:	GRANTED	
PRIMARY EXAMINER:	Travers, Russell	
ASSISTANT EXAMINER:	Hui, San-ming	
LEGAL REPRESENTATIVE:	Howson and Howson	
NUMBER OF CLAIMS:	16	
EXEMPLARY CLAIM:	1	
NUMBER OF DRAWINGS:	0 Drawing Figure(s); 0 Drawing Page(s)	
LINE COUNT:	3730	

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB This invention relates to cyclic combination therapies and regimens utilizing substituted indoline derivative compounds which are antagonists of the progesterone receptor having the general structure: ##STR1##

wherein R<sup>1</sup> and R<sup>2</sup> may be single substituents or fused to form spirocyclic rings, in combination with progestins, estrogens, or both. These methods of treatment may be used for contraception or for the treatment and/or prevention of secondary amenorrhea, dysfunctional bleeding, uterine leiomyomata, endometriosis; polycystic ovary syndrome, carcinomas and adenocarcinomas of the endometrium, ovary, breast, colon, prostate, or minimization of side effects or cyclic menstrual bleeding. Additional uses of the invention include stimulation of food intake.

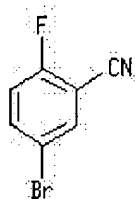
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 179897-89-3

(prepn. of oxospiro[cycloalkane-1,3'-indoline] derivs. and analogs as progesterone receptor antagonists)

RN 179897-89-3 USPATFULL

CN Benzonitrile, 5-bromo-2-fluoro- (9CI) (CA INDEX NAME)



L28 ANSWER 8 OF 59 USPATFULL on STN

Full  
Text

Chem  
References

ACCESSION NUMBER: 2002:259430 USPATFULL

TITLE: Monoamine reuptake inhibitors for treatment of CNS disorders

INVENTOR(S): Howard, Harry R., JR., Bristol, CT, UNITED STATES  
Schmidt, Christopher J., Old Lyme, CT, UNITED STATES  
Seeger, Thomas F., Mystic, CT, UNITED STATES

Elliott, Mark L., Canterbury, CT, UNITED STATES

	NUMBER	KIND	DATE	
<u>PATENT</u> INFORMATION:	US 2002143003	A1	20021003	<--
	US 6677378	B2	20040113	
<u>APPLICATION</u> INFO.:	US 2001-845992	A1	20010430	(9)
<u>RELATED</u> APPLN. INFO.:	Continuation-in-part of Ser. No. US 529207, PENDING A 371 of International Ser. No. WO 2000-IB108, filed on 2 Feb 2000, UNKNOWN			

	NUMBER	DATE
<u>PRIORITY</u> INFORMATION:	US 1999-121313P	19990223 (60)
DOCUMENT TYPE:	Utility	
FILE SEGMENT:	APPLICATION	
LEGAL REPRESENTATIVE:	Paul H. Ginsburg, Pfizer Inc., 20th Floor, 235 East 42nd Street, New York, NY, 10017-5755	
NUMBER OF CLAIMS:	15	
EXEMPLARY CLAIM:	1	
LINE COUNT:	1999	

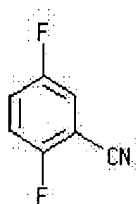
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB The present invention relates to compounds of the formula ##STR1##

wherein R<sup>1</sup> through R<sup>4</sup>, X, Y, m and n are defined as in the  
specification. Such compounds are useful exhibit activity as serotonin,  
norepinephrine and dopamine reuptake inhibitors, and their  
pharmaceutically acceptable salts, and their use in the treatment of  
central nervous system and other disorders.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 64248-64-2, 2,5-Difluorobenzonitrile  
(prepn. of phenoxybenzylamines as monoamine reuptake inhibitors)  
RN 64248-64-2 USPATFULL  
CN Benzonitrile, 2,5-difluoro- (9CI) (CA INDEX NAME)

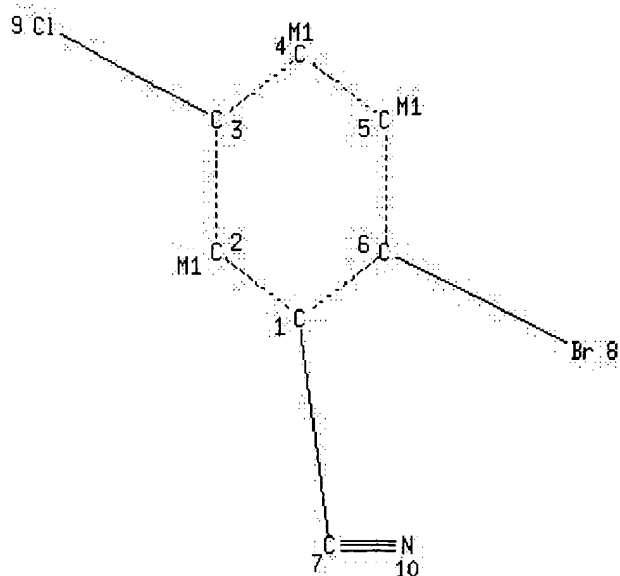


L28 ANSWER 9 OF 59 USPATFULL on STN

Full Text	Citing References
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ACCESSION NUMBER: 2002:243620 USPATFULL  
TITLE: 2,7-substituted octahydro-1H-pyrido[1,2-A]pyrazine  
derivatives as ligands for serotonin receptors  
INVENTOR(S): Desai, Kishor A., Ledyard, CT, UNITED STATES  
Fliri, Anton F., Stonington, CT, UNITED STATES  
Sanner, Mark A., Old Saybrook, CT, UNITED STATES

	NUMBER	KIND	DATE	
<u>PATENT</u> INFORMATION:	US 2002132811	A1	20020919	<--
<u>APPLICATION</u> INFO.:	US 2001-784567	A1	20010215	(9)
<u>RELATED</u> APPLN. INFO.:	Continuation of Ser. No. US 1999-368984, filed on 5 Aug			



## NODE ATTRIBUTES:

HCOUNT	IS	M1	AT	2
HCOUNT	IS	M1	AT	4
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NSPEC	IS	R	AT	1
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NSPEC	IS	C	AT	9
NSPEC	IS	C	AT	10

DEFAULT MLEVEL IS ATOM  
 MLEVEL IS CLASS AT 7 8 9 10  
 DEFAULT ECLEVEL IS LIMITED

## GRAPH ATTRIBUTES:

RSPEC I  
 NUMBER OF NODES IS 10

STEREO ATTRIBUTES: NONE

=> s 129

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 SAMPLE SCREEN SEARCH COMPLETED - 13 TO ITERATE

100.0% PROCESSED 13 ITERATIONS  
 SEARCH TIME: 00.00.01

1 ANSWERS

FULL FILE PROJECTIONS:	ONLINE	**COMPLETE**
	BATCH	**COMPLETE**
PROJECTED ITERATIONS:	44 TO	476
PROJECTED ANSWERS:	1 TO	80

L30 1 SEA SSS SAM L29

=> s 129 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS



DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y  
 FULL SEARCH INITIATED 14:24:03 FILE 'REGISTRY'  
 FULL SCREEN SEARCH COMPLETED - 295 TO ITERATE

100.0% PROCESSED 295 ITERATIONS 1 ANSWERS  
 SEARCH TIME: 00.00.01

L31 1 SEA SSS FUL L29

=> file hcaplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	155.84	834.15

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-14.70

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FILE COVERS 1907 - 1 Oct 2004 VOL 141 ISS 15  
 FILE LAST UPDATED: 30 Sep 2004 (20040930/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 131

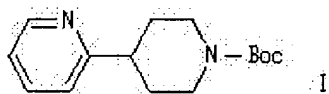
L32 4 L31

=> d 132, ibib abs fhitstr, 1-4

L32 ANSWER 1 OF 4 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text	Citing References
ACCESSION NUMBER:	2004:511300 HCAPLUS
DOCUMENT NUMBER:	141:174054
TITLE:	Direct synthesis of 4-arylpiperidines via palladium/copper(I)-cocatalyzed Negishi coupling of 4-piperidylzinc iodide with aromatic halides and triflates
AUTHOR(S):	Corley, Edward G.; Conrad, Karen; Murry, Jerry A.; Savarin, Cecile; Holko, Justin; Boice, Genevieve
CORPORATE SOURCE:	Departments of Process Research, and Chemical Engineering Research & Development, Merck Research Laboratories, Merck and Co., Inc., Rahway, NJ, 07065,

SOURCE: USA  
Journal of Organic Chemistry (2004), 69(15), 5120-5123  
CODEN: JOCEAH; ISSN: 0022-3263  
PUBLISHER: American Chemical Society  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI

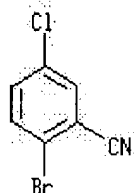


AB A general procedure for the synthesis of 4-arylpiperidines, e.g., I, via the coupling of 4-(N-Boc-piperidyl)zinc iodide with aryl halides and triflates is presented. The reaction required cocatalysis with both  $\text{Cl}_2\text{Pd}(\text{dppf})$  and a copper(I) species. An improved, safer procedure for the activation of zinc dust is also presented.

IT 57381-37-0, 2-Bromo-5-chlorobenzonitrile  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(prepn. of N-(Boc)-arylpiperidines via addn. of zinc to  
N-(Boc)-iodopiperidine followed by palladium/copper-catalyzed Negishi  
coupling with aryl halides and triflates)

RN 57381-37-0 HCAPLUS

CN Benzonitrile, 2-bromo-5-chloro- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L32 ANSWER 2 OF 4 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text	Citing References
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ACCESSION NUMBER: 2002:736258 HCAPLUS

DOCUMENT NUMBER: 137:263048

TITLE: Imidazo-pyrimidine derivatives as ligands for GABA receptors, and their preparation, pharmaceutical compositions, and use in the treatment of adverse neurological conditions.

INVENTOR(S): Chambers, Mark Stuart; Goodacre, Simon Charles; Hallett, David James; Jennings, Andrew; Jones, Philip; Lewis, Richard Thomas; Moore, Kevin William; Russell, Michael Geoffrey Neil; Street, Leslie Joseph; Szekeres, Helen Jane

PATENT ASSIGNEE(S): Merck Sharp & Dohme Limited, UK

SOURCE: PCT Int. Appl., 197 pp.

CODEN: PIXXD2

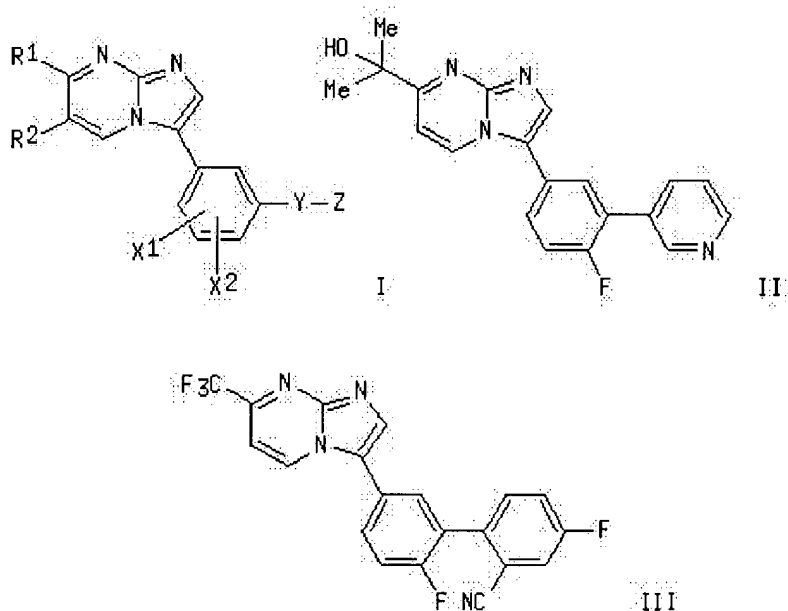
DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 3

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002074773	A1	20020926	WO 2002-GB1352	20020319
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2002193385	A1	20021219	US 2002-100797	20020319
EP 1381606	A1	20040121	EP 2002-706976	20020319
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
PRIORITY APPLN. INFO.:			GB 2001-7134	A 20010321
			GB 2001-27938	A 20011121
			US 2000-719712	A3 20001215
			WO 2002-GB1352	W 20020319
OTHER SOURCE(S): MARPAT 137:263048				
GI				



AB A class of 3-phenylimidazo[1,2-a]pyrimidine derivs. is disclosed. The compds. are substituted at the meta position of the Ph ring by an optionally substituted aryl or heteroaryl group, which is directly attached or bridged by an oxygen atom or an amino (NH) linkage, and which are further substituted on the Ph ring by alkyl, CF<sub>3</sub>, alkoxy, or one or two halogen atoms, esp. fluoro. The compds. are selective ligands for GABAA receptors, in particular having good affinity for the  $\alpha 2$  and/or  $\alpha 3$  and/or  $\alpha 5$  subunit thereof, and are accordingly of benefit in the treatment and/or prevention of adverse conditions of the central nervous system, including anxiety, convulsions, and cognitive disorders. In particular, the compds. are represented by I [wherein X1 = halo, C1-6 alkyl, CF<sub>3</sub>, or C1-6 alkoxy; X2 = H or halo; Y = bond, O, or NH;

Z = (un)substituted aryl or heteroaryl; R1 = H, hydrocarbyl, heterocyclyl, halo, cyano, CF3, NO2, ORa, SRa, SORa, SO2Ra, SO2NRaRb, NRaRb, NRaCORb, NRaCO2Rb, CORa, CO2Ra, CONRaRb, or CRa:NORb; R2 = H or halo; Ra, Rb = H, hydrocarbyl, or heterocyclyl], and include their salts and prodrugs. For instance, 3-hydroxy-3-methyl-2-butanone was O-acetylated, condensed with tri-Et orthoformate, and then cyclocondensed with 2-aminoimidazole hemisulfate to give 2-(imidazo[1,2-a]pyrimidin-7-yl)propan-2-ol. This compd. underwent ring bromination in the 3-position, followed by Pd(0)-catalyzed coupling of the bromide with 3-[2-fluoro-5-(4,4,5,5-tetramethyl-[1,3,2]dioxaborolan-2-yl)phenyl]pyridine, to give preferred title compd. II, isolated as the di-HCl salt. Another preferred compd., III, was prepd. via coupling of 3-bromo-7-trifluoromethylimidazo[1,2-a]pyrimidine with 5'-(5,5-dimethyl-[1,3,2]dioxaborinan-2-yl)-4,2'-difluorobiphenyl-2-carbonitrile (preps. given). I potently inhibited the binding of [3H]-flumazenil to the benzodiazepine binding site of human GABAA receptors contg.  $\alpha 2$  and/or  $\alpha 3$  and/or  $\alpha 5$  subunits (stably expressed in Ltk- cells), with all example compds. showing a  $K_i$  of 100 nM or less.

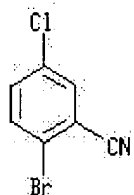
IT **57381-37-0P**, 2-Bromo-5-chlorobenzonitrile

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; prepn. of imidazopyrimidine derivs. as GABAA receptor ligands for use as anxiolytics, anticonvulsants, and cognition enhancers)

RN 57381-37-0 HCAPLUS

CN Benzonitrile, 2-bromo-5-chloro- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L32 ANSWER 3 OF 4 HCAPLUS COPYRIGHT 2004 ACS on STN

Full  
Text

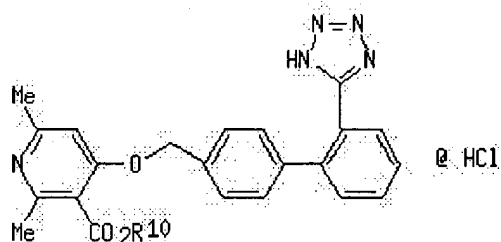
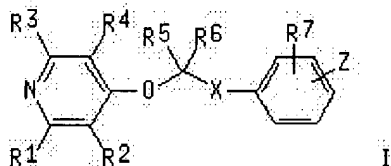
Citing  
References

ACCESSION NUMBER: 1992:59379 HCAPLUS  
DOCUMENT NUMBER: 116:59379  
TITLE: Preparation of 4-(tetrazolylbiphenylmethoxy)pyridine  
s and related compounds as angiotensin II antagonists  
INVENTOR(S): Roberts, David Anthony; Bradbury, Robert Hugh;  
Ratcliffe, Arnold Harry  
PATENT ASSIGNEE(S): Imperial Chemical Industries PLC, UK  
SOURCE: Eur. Pat. Appl., 55 pp.  
CODEN: EPXXDW  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 453210	A2	19911023	EP 1991-303300	19910415
EP 453210	A3	19930113		

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE

<u>GB 2244054</u>	A1	19911120	<u>GB 1991-8081</u>	19910415
<u>GB 2244054</u>	B2	19940406		
<u>CA 2040747</u>	AA	19911020	<u>CA 1991-2040747</u>	19910418
<u>NO 9101534</u>	A	19911021	<u>NO 1991-1534</u>	19910418
<u>AU 9175083</u>	A1	19911024	<u>AU 1991-75083</u>	19910418
<u>ZA 9102912</u>	A	19911224	<u>ZA 1991-2912</u>	19910418
<u>US 5130318</u>	A	19920714	<u>US 1991-687270</u>	19910418
<u>JP 06199796</u>	A2	19940719	<u>JP 1991-228211</u>	19910418
<u>JP 3120873</u>	B2	20001225		
<u>FI 9101924</u>	A	19911020	<u>FI 1991-1924</u>	19910419
<u>CN 1055925</u>	A	19911106	<u>CN 1991-102514</u>	19910419
<u>HU 57206</u>	A2	19911128	<u>HU 1991-1295</u>	19910419
<u>US 5198439</u>	A	19930330	<u>US 1992-874785</u>	19920427
<u>PRIORITY APPLN. INFO.:</u>			<u>GB 1990-8817</u>	A 19900419
			<u>GB 1990-26617</u>	A 19901207
			<u>US 1991-687270</u>	A3 19910418
OTHER SOURCE(S):			MARPAT 116:59379	
GI				



AB Title compds. [I; R1 = H, (cyclo)alkyl, Ph, substituted alkyl; R2 = H, (cyclo)alkyl, cycloalkylalkyl, CO<sub>2</sub>H, alkoxy carbonyl, cyano, NO<sub>2</sub>, Ph, phenylalkyl; R3 = halo, alkoxy, amino, R1; R4 = H, (substituted) alkyl, carboxy, alkoxy carbonyl, cyano, NO<sub>2</sub>, carbamoyl, halo, amino, acylamino, etc.; R3R4 = (CO-interrupted) alkylene, alkenylene; R5 = H; R6 = H, alkyl; R7 = R6, alkoxy, halo, CF<sub>3</sub>, cyano, NO<sub>2</sub>; X = (substituted) phenylene, bond; Z = tetrazolyl, tetrazolylaminocarbonyl, etc.; and N-oxides thereof], were prepd. Thus, Et 1,4-dihydro-2,6-dimethyl-4-oxopyridine-3-carboxylate was condensed with 5-[2-(4'-bromomethylbiphenyl)]-2-triphenylmethyl-2H-tetrazole using NaH in DMF and the product was detritylated with 6 M HCl in dioxane to give title compd. II (R<sub>10</sub> = Et). II (R<sub>10</sub> = Me) in rats antagonized angiotensin II with IC<sub>50</sub> = 0.1 mg/kg i.v.

IT **57381-37-0P**

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of, as intermediate for angiotensin II antagonists)

RN 57381-37-0 HCAPLUS

CN Benzonitrile, 2-bromo-5-chloro- (9CI) (CA INDEX NAME)

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
 BATCH \*\*COMPLETE\*\*  
 PROJECTED ITERATIONS: 119 TO 641  
 PROJECTED ANSWERS: 0 TO 0

L34 0 SEA SSS SAM L33

=> s l33 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS  
 DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y  
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 FULL SCREEN SEARCH COMPLETED - 461 TO ITERATE

100.0% PROCESSED 461 ITERATIONS 1 ANSWERS  
 SEARCH TIME: 00.00.01

L35 1 SEA SSS FUL L33

=> file hcaplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	156.26	1011.81

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FILE COVERS 1907 - 1 Oct 2004 VOL 141 ISS 15  
 FILE LAST UPDATED: 30 Sep 2004 (20040930/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l35

L36 4 L35

=> d l36, ibib abs fhitr, 1-4

L36 ANSWER 1 OF 4 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text	Citing References
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ACCESSION NUMBER: 2002:669675 HCAPLUS  
 DOCUMENT NUMBER: 137:201317

TITLE: Preparation of benzoxazinone cyclic carbamate antiprogestins for use in combination therapies and regimens with progestational agents.

INVENTOR(S): Grubb, Gary S.; Zhang, Puwen; Terefenko, Eugene A.; Fensome, Andrew; Wrobel, Jay E.; Fletcher, Iii Horace; Edwards, James P.; Jones, Todd K.; Tegley, Christopher M.; Zhi, Lin

PATENT ASSIGNEE(S): Wyeth, John and Brother Ltd., USA; Ligand Pharmaceuticals Incorporated

SOURCE: U.S., 44 pp.  
CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 3

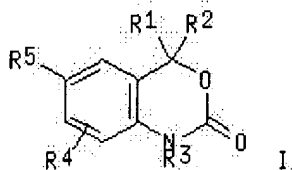
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6444668	B1	20020903	US 2000-552350	20000419
JP 2002543155	T2	20021217	JP 2000-615048	20000501
US 2003045511	A1	20030306	US 2002-141792	20020509
US 6759408	B2	20040706		

PRIORITY APPLN. INFO.:

US 1999-229346P	P	19990504
US 1999-304712	A	19990504
US 2000-552350	A	20000419
WO 2000-US11643	W	20000501

OTHER SOURCE(S): MARPAT 137:201317  
GI



AB A method of contraception comprises administration to a female of a progestational agent in a first phase and in a second phase administration of [I; R1, R2 = H, (un)substituted C1-6 alkyl, C2-6 alkenyl, C2-6 alkynyl, C3-8 cycloalkyl, aryl, heterocyclyl, amino deriv.; R1R2 = atoms to form spirocyclic or heterospirocyclic rings; R3 = H, OH, NH2, (un)substituted C1-6 alkyl, C3-6 alkenyl, alkynyl, COR6; R6 = H, (un)substituted C1-3 alkyl, aryl, C1-3 alkoxy, C1-3 aminoalkyl; R4 = H, halo, CN, NO2, (un)substituted C1-6 alkyl, alkynyl, C1-6 alkoxy, amino, C1-6 aminoalkyl; R5 = trisubstituted benzene ring, 5-6 membered ring with 1, 2, or 3 O, S, SO, SO2, NR7 and contg. 1-2 H, halo, CN, NO2, amino, C1-3 alkyl, C1-3 alkoxy, C1-3 aminoalkyl, COR8, NR9COR8; R7 = H, C1-3 alkyl; R8 = H, (un)substituted C1-3 alkyl, aryl, C1-3 alkoxy, C1-3 aminoalkyl; R9 = H, (un)substituted C1-3 alkyl]. Thus, 6-(3-chlorophenyl)-4,4-dimethyl-1,4-dihydrobenzo[d][1,3]-oxazin-2-one was prepd. from 2-(2-amino-5-bromophenyl)propan-2-ol via cyclocondensation with 1,1-carbonyldiimidazole followed by palladium-catalyzed coupling with 3-chlorophenylboronic acid. I demonstrated IC50's of 2.7-68 nM in a hPR decidualization assay.

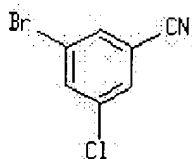
IT 304854-55-5, Benzonitrile, 3-bromo-5-chloro-

RL: RCT (Reactant); RACT (Reactant or reagent)

(prepn. of benzoxazinone cyclic carbamate antiprogestins for use in combination therapies and regimens with progestational agents)

RN 304854-55-5 HCAPLUS

CN Benzonitrile, 3-bromo-5-chloro- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 75 THERE ARE 75 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L36 ANSWER 2 OF 4 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text      Citations  
References

ACCESSION NUMBER: 2000:790489 HCAPLUS  
DOCUMENT NUMBER: 133:350229  
TITLE: Novel cyclocarbamate derivatives as progesterone receptor modulators  
INVENTOR(S): Zhang, Puwen; Terefenko, Eugene A.; Fletcher, Horace, III; Fensome, Andrew; Wrobel, Jay E.; Zhi, Lin; Jones, Todd K.; Marschke, Keith B.; Tegley, Christopher M.  
PATENT ASSIGNEE(S): American Home Products Corporation, USA; Ligand Pharmaceuticals, Inc.  
SOURCE: PCT Int. Appl., 135 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

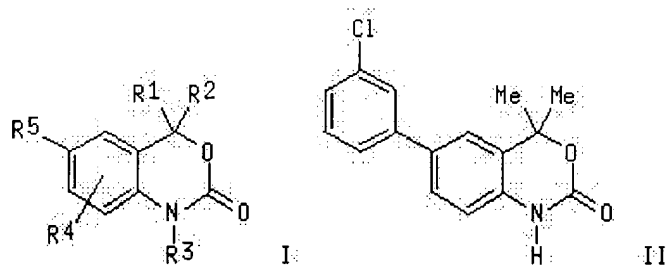
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000066571	A1	20001109	WO 2000-US11822	20000501
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
US 6509334	B1	20030121	US 2000-552633	20000419
EP 1173426	A1	20020123	EP 2000-928689	20000501
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
BR 2000010213	A	20020219	BR 2000-10213	20000501
TR 200103286	T2	20020722	TR 2001-200103286	20000501
JP 2002543193	T2	20021217	JP 2000-615601	20000501
AU 766428	B2	20031016	AU 2000-46886	20000501
NZ 515355	A	20040227	NZ 2000-515355	20000501
US 2002049204	A1	20020425	US 2001-948309	20010906
US 6566358	B2	20030520		
ZA 2001007630	A	20020514	ZA 2001-7630	20010917
NO 2001005378	A	20020103	NO 2001-5378	20011102
BG 106079	A	20020531	BG 2001-106079	20011102
US 2003216388	A1	20031120	US 2003-386799	20030312
US 6713478	B2	20040330		
US 2004186101	A1	20040923	US 2004-767813	20040129
PRIORITY APPLN. INFO.:			US 1999-183012P	P 19990504



US 2000-552633  
 WO 2000-US11822  
 US 2001-948309  
 US 2003-386799

A1 20000419  
 W 20000501  
 A3 20010906  
 A1 20030312

OTHER SOURCE(S): MARPAT 133:350229  
 GI



AB This invention discloses novel aryl fused cyclocarbamate derivs. I (R1 or R2 = H, (un)substituted C1-6 alkyl, (un)substituted C2-6 alkenyl, (un)substituted C2-6 alkynyl, (un)substituted C3-8 cycloalkyl, (un)substituted aryl, (un)substituted heterocyclyl, amino deriv. or R1 and R2 may be fused to form spirocyclic or heterospirocyclic rings; R3 = H, OH, NH2, (un)substituted C1-6 alkyl, (un)substituted C3-6 alkenyl, (un)substituted alkynyl, or COR6 {R6 = H, (un)substituted C1-3 alkyl, (un)substituted aryl, (un)substituted C1-3 alkoxy, or (un)substituted C1-3 aminoalkyl}; R4 = H, halo, CN, NO2, (un)substituted C1-6 alkyl, (un)substituted alkynyl, (un)substituted C1-6 alkoxy, amino, or (un)substituted C1-6 aminoalkyl; R5 = trisubstituted benzene ring or a five- or six-membered ring with 1, 2, or 3 heteroatoms selected from O, S, SO, SO2 or NR7 and contg. one or two independent substituents from the group including H, halo, CN, NO2, amino, C1-3 alkyl, C1-3 alkoxy, C1-3 aminoalkyl, COR8, or NR9COR8 {R7 = H or C1-3 alkyl; R8 = H, (un)substituted C1-3 alkyl, (un)substituted aryl, (un)substituted C1-3 alkoxy or (un)substituted C1-3 aminoalkyl; R9 = H, (un)substituted C1-3 alkyl}) or pharmaceutically acceptable salts thereof, as well as pharmaceutical compns. and methods using the compds. as antagonists of the progesterone receptor. Thus, cyclocarbamate II was prepd. from 2-(2-amino-5-bromophenyl)propan-2-ol via cyclocondensation with 1,1-carbonyldiimidazole followed by palladium-catalyzed coupling with 3-chlorophenylboronic acid. Compds. of the invention demonstrated potency in the range of 0.01 nM to 5  $\mu$ M in the in vitro assays, and 0.001 to 300 mg/kg in the in vivo assays.

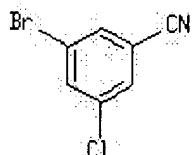
IT 304854-55-5

RL: RCT (Reactant); RACT (Reactant or reagent)

(prepn. of benzooxazinone derivs. as progesterone receptor modulators)

RN 304854-55-5 HCAPLUS

CN Benzonitrile, 3-bromo-5-chloro- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

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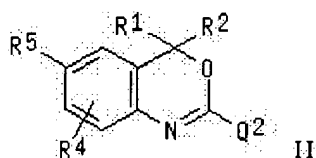
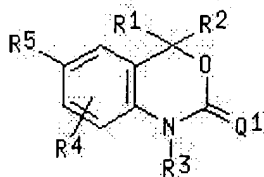
THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

Full Text	Citing References
--------------	----------------------

ACCESSION NUMBER: 2000:790488 HCAPLUS  
 DOCUMENT NUMBER: 133:350228  
 TITLE: Preparation of cyclothiocarbamate derivatives as  
 progesterone receptor modulators  
 INVENTOR(S): Zhang, Puwen; Fensome, Andrew; Terefenko, Eugene A.;  
 Zhi, Lin; Jones, Todd K.; Marschke, Keith B.; Tegley,  
 Christopher M.  
 PATENT ASSIGNEE(S): American Home Products Corporation, USA; Ligand  
 Pharmaceuticals, Inc.  
 SOURCE: PCT Int. Appl., 101 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000066570	A1	20001109	WO 2000-US11749	20000501
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
US 6436929	B1	20020820	US 2000-552354	20000419
EP 1175411	A1	20020130	EP 2000-930266	20000501
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
BR 2000010214	A	20020213	BR 2000-10214	20000501
TR 200103285	T2	20020221	TR 2001-200103285	20000501
JP 2002543192	T2	20021217	JP 2000-615600	20000501
AU 766801	B2	20031023	AU 2000-48119	20000501
CN 1131856	B	20031224	CN 2000-807099	20000501
NZ 515353	A	20040326	NZ 2000-515353	20000501
ZA 2001007633	A	20020514	ZA 2001-7633	20010917
NO 2001005381	A	20020103	NO 2001-5381	20011102
BG 106080	A	20020531	BG 2001-106080	20011102
US 2003092711	A1	20030515	US 2002-140034	20020506
PRIORITY APPLN. INFO.:			US 1999-183013P	P 19990504
			US 2000-552354	A1 20000419
			WO 2000-US11749	W 20000501

OTHER SOURCE(S): MARPAT 133:350228  
 GI



AB The title compds. [I or II; R1, R2 = H, alkyl, alkenyl, etc.; or R1 and R2  
 are fused to form (un)substituted 3-8 membered spiro cyclic alkyl or

alkenyl ring or a spiro cyclic ring contg. 1-3 heteroatoms selected from O, S and N; R3 = H, OH, NH2, etc.; R4 = H, halo, CN, etc.; R5 = (un)substituted Ph, 5-6 membered heterocyclic ring with 1-3 ring heteroatoms, 3-pyridyl, 5-pyrimidinyl; Q1 = S, NR7, CR8R9; R7 = CN, alkyl, cycloalkyl, etc.; R8, R9 = H, alkyl, cycloalkyl, etc.; Q2 = NR11OR12, NR11NR12R13, ONR11R13; R11-R13 = H, alkyl, aryl, etc.] which are agonists of the progesterone receptor, and are useful for contraception and the treatment of progesterone-related maladies, were prepd. E.g., a multi-step synthesis of I [R1, R2 = Me; R3, R4 = H; R5 = 3-ClC6H4; Q1 = S] which showed EC50 of 0.65 nM against hPR in CV-1 cells, was given.

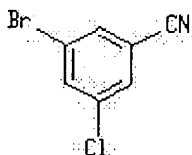
IT **304854-55-5**

RL: RCT (Reactant); RACT (Reactant or reagent)

(prepn. of cyclothiocarbamate derivs. as progesterone receptor modulators)

RN **304854-55-5** HCAPLUS

CN Benzonitrile, 3-bromo-5-chloro- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

5

THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L36 ANSWER 4 OF 4 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text	Cited References
ACCESSION NUMBER:	2000:790347 HCAPLUS
DOCUMENT NUMBER:	133:350205
TITLE:	Contraceptive compositions containing antiprogesterone and progestinic dihydro-2H-3,1-benzoxazin-2-ones
INVENTOR(S):	Grubb, Gary S.; Zhi, Lin; Jones, Todd K.; Marschke, Keith B.; Tegley, Christopher M.
PATENT ASSIGNEE(S):	American Home Products Corporation, USA; Ligand Pharmaceuticals, Inc.
SOURCE:	PCT Int. Appl., 146 pp.
DOCUMENT TYPE:	Patent
LANGUAGE:	English
FAMILY ACC. NUM. COUNT:	3
PATENT INFORMATION:	

ACCESSION NUMBER: 2000:790347 HCAPLUS

DOCUMENT NUMBER: 133:350205

TITLE: Contraceptive compositions containing antiprogesterone and progestinic dihydro-2H-3,1-benzoxazin-2-ones

INVENTOR(S): Grubb, Gary S.; Zhi, Lin; Jones, Todd K.; Marschke, Keith B.; Tegley, Christopher M.

PATENT ASSIGNEE(S): American Home Products Corporation, USA; Ligand Pharmaceuticals, Inc.

SOURCE: PCT Int. Appl., 146 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 3

PATENT INFORMATION:

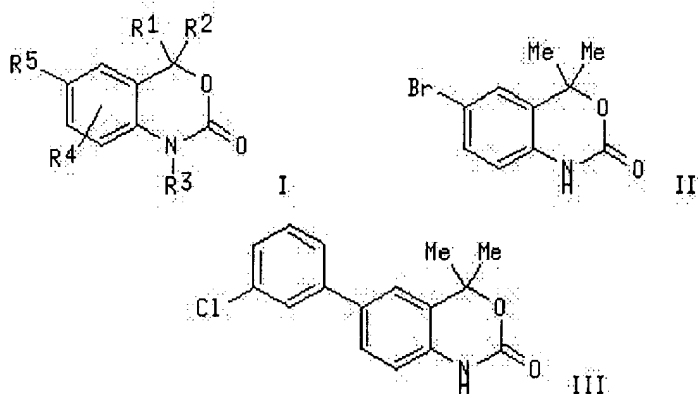
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000066164	A1	20001109	WO 2000-US11643	20000501
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
US 6498154	B1	20021224	US 2000-552357	20000419
EP 1173210	A1	20020123	EP 2000-928611	20000501
EP 1173210	B1	20040915		

103/21

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,  
IE, SI, LT, LV, FI, RO

JP 2002543155	T2	20021217	JP 2000-615048	20000501
PRIORITY APPLN. INFO.:			US 1999-304712	A 19990504
			US 2000-552357	A1 20000419
			US 1999-183042P	P 19990504
			US 2000-552350	A 20000419
			WO 2000-US11643	W 20000501

OTHER SOURCE(S): MARPAT 133:350205  
GI



AB The dihydrobenzoxazinones I [R1, R2 = H, alkyl, alkenyl, alkynyl, cycloalkyl, aryl, heterocyclyl, acyl, acylamino; or R1R2 are fused to form spirocyclic or hetero-spirocyclic rings substituted by F, alkyl, alkoxy, alkylthio, F3C, HO, cyano, H2N, alkylamino; R3 = H, OH, NH2, C1-6 alkyl, C3-6 alkenyl, alkynyl, CORC; RC = H, C1-3 alkyl, aryl, C1-3 alkoxy, C1-3 aminoalkyl; R4 = H, halo, cyano, NO2, alkyl, alkynyl, alkoxy, alkoxy, amino, aminoalkyl; R5 = XYZC6H2, X = halo, cyano, alkyl, alkenyl, alkynyl, alkoxy, thioalkoxy, H2N, aminoalkyl, NO2, perfluoroalkyl, 5- or 6-membered heterocyclyl; Y, Z = H, halo, cyano, NO2, H2N, aminoalkyl, alkoxy, alkyl, thioalkoxy; or R5 = 5- or 6-membered heterocyclyl with O, S, SO, SO2 heteroatoms substituted by H, halo, cyano, NO2, H2N, alkyl, alkoxy, perfluoroacyl, perfluoroacylamino] and their pharmaceutically acceptable salts were prepd. as antagonists of the progesterone receptor and were useful to induce contraception in mammals in cyclic combination therapies using an antiprogesterone and progesterone where the progesterone is administered in the alternating presence and absence of an antiprogesterone. These methods of treatment may be used for contraception or for the treatment and/or prevention of secondary amenorrhea, dysfunctional bleeding, uterine leiomyomata, endometriosis; polycystic ovary syndrome, carcinomas and adenocarcinomas of the endometrium, ovary, breast, colon, prostate, or minimization of side effects of cyclic menstrual bleeding. Addnl. uses of the invention include stimulation of food intake. Thus, cyclocondensation of 2-(2-amino-5-bromophenyl)-2-propanol with carbonyldiimidazole gave the dimethylbenzoxazinone II which coupled with 3-chlorophenylboronic acid in DME/H2O contg. (Ph3P)4Pd and Na2CO3 to give the (chlorophenyl)benzoxazinone III.

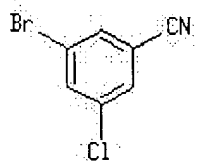
IT **304854-55-5**

RL: RCT (Reactant); RACT (Reactant or reagent)

(prepn. of substituted dihydrobenzoxazinones with progesterone receptor antagonist activity for use in contraceptive compns.)

RN **304854-55-5** HCAPLUS

CN Benzonitrile, 3-bromo-5-chloro- (9CI) (CA INDEX NAME)

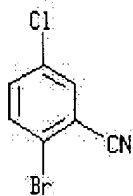


REFERENCE COUNT:

6

THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=>



L32 ANSWER 4 OF 4 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text	Chemical References
--------------	------------------------

ACCESSION NUMBER: 1975:606332 HCAPLUS  
 DOCUMENT NUMBER: 83:206332  
 TITLE: Benzoguanamine derivatives  
 INVENTOR(S): Murai, Hiromu; Ohata, Katsuya; Aoyagi, Yoshiaki; Ueda, Fusao; Kitano, Masahiko; Takata, Satoshi; Tada, Shinichi  
 PATENT ASSIGNEE(S): Nippon Shinyaku Co., Ltd., Japan  
 SOURCE: Ger. Offen., 24 pp.  
 CODEN: GWXXBX  
 DOCUMENT TYPE: Patent  
 LANGUAGE: German  
 FAMILY ACC. NUM. COUNT: 3  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2506814	A1	19750828	DE 1975-2506814	19750218
DE 2506814	C3	19791115		
DE 2506814	B2	19790322		
JP 50111085	A2	19750901	JP 1974-19211	19740218
JP 55004751	B4	19800131		
JP 50111086	A2	19750901	JP 1974-19212	19740218
JP 52046955	B4	19771129		
US 3966728	A	19760629	US 1975-544176	19750127
CH 592639	A	19771031	CH 1975-1301	19750204
CH 592638	A	19771031	CH 1975-1300	19750204
SE 7501273	A	19750819	SE 1975-1273	19750205
SE 425245	B	19820913	SE 1975-1274	19750205
SE 425245	C	19821230		
DK 7500436	A	19751020	DK 1975-436	19750207
DK 138268	C	19790212		
DK 138116	B	19780717	DK 1975-437	19750207
DK 138116	C	19781204		
NL 7501574	A	19750820	NL 1975-1574	19750211
NL 157901	B	19780915		
NL 157902	B	19780915	NL 1975-1575	19750211
FR 2261009	A1	19750912	FR 1975-4690	19750214
BE 825673	A1	19750616	BE 1975-153471	19750218
AT 7501200	A	19770315	AT 1975-1200	19750218
AT 339909	B	19771110		
AT 7501197	A	19770515	AT 1975-1197	19750218
AT 340941	B	19780110		
PRIORITY APPLN. INFO.:			JP 1974-19211	19740218
			JP 1974-19212	19740218

GI For diagram(s), see printed CA Issue.

AB Triazines I (R = 2-Cl, 2-F, 2-Br, 3-Cl, R1 = 5-Cl; R = 2-Cl, R1 = 5-Br, 4-Cl, 3-Cl, 6-Cl, 5-F; R = 2-Br, 2-F, R1 = 5-F, 5-Br, 4-Cl; R = 3-Cl, R1 = 4-Br) were prepd. by treating RR1C6H3CN with dicyandiamide or dihalobenzoic acid derivs. with biguanide. I inhibit ulceration. Thus 20

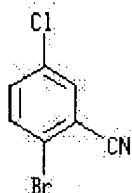
mg/kg I (R = 2-Cl, R1 = 5-Cl) i.p. in rats gave total inhibition of Shay ulcers.

IT **57381-37-0**

RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with dicyanamide)

RN 57381-37-0 HCAPLUS

CN Benzonitrile, 2-bromo-5-chloro- (9CI) (CA INDEX NAME)



=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	21.40	855.55
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-2.80	-17.50

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STRUCTURE FILE UPDATES: 29 SEP 2004 HIGHEST RN 754169-63-6  
DICTIONARY FILE UPDATES: 29 SEP 2004 HIGHEST RN 754169-63-6

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

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Crossover limits have been increased. See [HELP CROSSOVER](#) for details.

Experimental and calculated property data are now available. For more information enter [HELP PROP](#) at an arrow prompt in the file or refer to the file summary sheet on the web at:  
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=>

L33 STRUCTURE UPLOADED

=> s l33

SAMPLE SEARCH INITIATED 14:26:12 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 19 TO ITERATE

100.0% PROCESSED 19 ITERATIONS 0 ANSWERS  
SEARCH TIME: 00.00.01

1999, GRANTED, Pat. No. US 6231833 Continuation-in-part of Ser. No. US 1998-135946, filed on 18 Aug 1998, ABANDONED Continuation-in-part of Ser. No. US 1997-809145, filed on 26 Mar 1997, GRANTED, Pat. No. US 5852031 Continuation-in-part of Ser. No. WO 1995-IB689, filed on 24 Aug 1995, UNKNOWN Continuation of Ser. No. US 1994-315470, filed on 30 Sep 1994, ABANDONED

DOCUMENT TYPE: Utility  
FILE SEGMENT: APPLICATION  
LEGAL REPRESENTATIVE: PFIZER INC, 150 EAST 42ND STREET, 5TH FLOOR - STOP 49, NEW YORK, NY, 10017-5612  
NUMBER OF CLAIMS: 36  
EXEMPLARY CLAIM: 1  
LINE COUNT: 2614

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

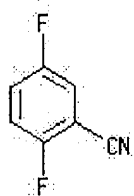
AB Substituted pyrido[1,2-a]pyrazines of general formula I; wherein Ar and Ar<sup>1</sup> represent various carbocyclic and heterocyclic aromatic rings; A represents O, S, SO, SO<sub>2</sub>, CHOH, C.dbd.O, or --(CR<sup>3R4</sup>); and n is 0-2, as well as precursors thereof, are ligands for dopamine receptor subtypes and serotonin (5HT) within the body and are therefore useful in the treatment of disorders of the dopamine and serotonin systems: ##STR1##

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 64248-64-2, 2,5-Difluorobenzonitrile  
(prepn. of N-aryloctahydro-1H-pyrido[1,2-a]pyrazines as dopamine receptor ligands)

RN 64248-64-2 USPATFULL

CN Benzonitrile, 2,5-difluoro- (9CI) (CA INDEX NAME)



L28 ANSWER 10 OF 59 USPATFULL on STN

Full  
Text

Citing  
References

ACCESSION NUMBER: 2002:224612 USPATFULL  
TITLE: Combination regimens using progesterone receptor modulators  
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	NUMBER	KIND	DATE	
PATENT INFORMATION:	US 6444668	B1	20020903	<--
APPLICATION INFO.:	US 2000-552350		20000419	(9)

	NUMBER	DATE
PRIORITY INFORMATION:	US 1999-229346P	19990504 (60)
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FILE SEGMENT:	GRANTED	
PRIMARY EXAMINER:	Travers, Russell	
ASSISTANT EXAMINER:	Wang, Shengjun	
LEGAL REPRESENTATIVE:	Howson and Howson	
NUMBER OF CLAIMS:	29	
EXEMPLARY CLAIM:	1	
NUMBER OF DRAWINGS:	0 Drawing Figure(s); 0 Drawing Page(s)	
LINE COUNT:	4086	

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB This invention relates to cyclic combination therapies and regimens utilizing substituted indoline derivative compounds which are antagonists of the progesterone receptor having the general structure:  
##STR1##

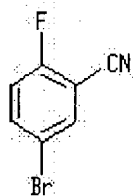
wherein R<sup>1</sup> and R<sup>2</sup> may be single substituents or fused to form spirocyclic or hetero-spirocyclic rings; R<sup>3</sup> is H, OH, NH<sub>2</sub>, C<sub>1</sub> to C<sub>6</sub> alkyl, substituted C<sub>1</sub> to C<sub>6</sub> allyl C<sub>3</sub> to C<sub>6</sub> alkenyl, substituted C<sub>1</sub> to C<sub>6</sub> alkenyl, alkynyl, or substituted alknyl, COR<sup>C</sup>; R<sup>C</sup> is H, C<sub>1</sub> to C<sub>3</sub> alkyl, substituted C<sub>1</sub> to C<sub>3</sub> alkyl, aryl, substituted aryl, C<sub>1</sub> to C<sub>3</sub> alkoxy, substituted C<sub>1</sub> to C<sub>3</sub> alkoxy, C<sub>1</sub> to C<sub>3</sub> aminoalkyl, or substituted C<sub>1</sub> to C<sub>3</sub> aminoalkyl; R<sup>4</sup> is H, halogen, CN, NO<sub>2</sub>, C<sub>1</sub> to C<sub>6</sub> alkyl, substituted C<sub>1</sub> to C<sub>6</sub> alkyl alkynyl, or substituted alkynyl, C<sub>1</sub> to C<sub>6</sub> alkoxy, substituted C<sub>1</sub> to C<sub>6</sub> alkoxy, amino, C<sub>1</sub> to C<sub>6</sub> aminoalkyl, or substituted C<sub>1</sub> to C<sub>6</sub> aminoalkyl; and R<sup>5</sup> is selected from a trisubstituted benzene ring of a five or six membered ring with 1, 2, or 3 heteroatoms from the group including O, S, SO, SO<sub>2</sub> or NR<sup>6</sup> and containing one or two independent substituents from the group including H, halogen, CN, NO<sub>2</sub>, amino, and C<sub>1</sub> to C<sub>3</sub> alkyl, C<sub>1</sub> to C<sub>3</sub> alkoxy, C<sub>1</sub> to C<sub>3</sub> aminoalkyl, COR<sup>F</sup>, or NR<sup>G</sup>COR<sup>F</sup>; or pharmaceutically acceptable salt thereof. These methods of treatment may be used for contraception or for the treatment and/or prevention of secondary amenorrhea, dysfunctional bleeding, uterine leiomyomata, endometriosis; polycystic ovary syndrome, carcinomas and adenocarcinomas of the endometrium, ovary, breast, colon, prostate, or innmization of side effects or cyclic menstrual bleeding. Additional uses of the invention include stimulation of food intake.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 179897-89-3, Benzonitrile, 5-bromo-2-fluoro-  
(prepn. of benzoxazinone cyclic carbamate antiprogestins for use in combination therapies and regimens with progestational agents)

RN 179897-89-3 USPATFULL

CN Benzonitrile, 5-bromo-2-fluoro- (9CI) (CA INDEX NAME)



=> file reg

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
84.63	678.31

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
0.00	-14.70

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STRUCTURE FILE UPDATES: 29 SEP 2004 HIGHEST RN 754169-63-6

DICTIONARY FILE UPDATES: 29 SEP 2004 HIGHEST RN 754169-63-6

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:  
<http://www.cas.org/ONLINE/DBSS/registryss.html>

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L29 STRUCTURE UPLOADED

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L29 HAS NO ANSWERS

L29 STR